

FILE 'REGISTRY' ENTERED AT 09:29:25 ON 10 DEC 2008
 L1 STRUCTURE UPLOADED
 L2 50 S L1
 L3 15948 S L1 SSS FULL

FILE 'HCAPLUS' ENTERED AT 09:30:58 ON 10 DEC 2008
 L4 6873 S L3

FILE 'REGISTRY' ENTERED AT 09:31:10 ON 10 DEC 2008
 L5 STRUCTURE UPLOADED
 L6 45 S L5
 L7 6574 S L5 SSS FULL
 L8 9374 S L3 NOT L7
 L9 STRUCTURE UPLOADED
 L10 50 S L9
 L11 5859 S L9 SSS FULL
 L12 3518 S L8 NOT L11

FILE 'HCAPLUS' ENTERED AT 09:34:25 ON 10 DEC 2008
 L13 1452 S L12
 L14 1009 S L12/PREP

FILE 'REGISTRY' ENTERED AT 09:34:50 ON 10 DEC 2008
 L15 STRUCTURE UPLOADED
 L16 STRUCTURE UPLOADED
 L17 STRUCTURE UPLOADED
 L18 135 S L15 SUB=L12 FULL
 L19 818 S L16 SUB=L12 FULL
 L20 1352 S L17 SUB=L12 FULL
 L21 3383 S L12 NOT L18
 L22 2567 S L21 NOT L19
 L23 1221 S L22 NOT L20

FILE 'HCAPLUS' ENTERED AT 09:40:15 ON 10 DEC 2008
 L24 740 S L23
 L25 561 S L23/PREP

FILE 'STNGUIDE' ENTERED AT 09:40:30 ON 10 DEC 2008

FILE 'REGISTRY' ENTERED AT 09:45:51 ON 10 DEC 2008
 L26 STRUCTURE UPLOADED
 L27 1024 S L26 SUB=L23 FULL
 L28 STRUCTURE UPLOADED
 L29 12 S L28 SUB=L27 FULL
 L30 STRUCTURE UPLOADED
 L31 110 S L30 SUB=L27 FULL

FILE 'HCAPLUS' ENTERED AT 09:49:12 ON 10 DEC 2008
 L32 52 S L31
 L33 42 S L32 AND (PY<2003 OR AY<2003 OR PRY<2003)

```
=> file registry
COST IN U.S. DOLLARS                SINCE FILE      TOTAL
                                     ENTRY      SESSION
FULL ESTIMATED COST                0.21      0.21
```

FILE 'REGISTRY' ENTERED AT 09:29:25 ON 10 DEC 2008
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STRUCTURE FILE UPDATES: 8 DEC 2008 HIGHEST RN 1082116-14-0
DICTIONARY FILE UPDATES: 8 DEC 2008 HIGHEST RN 1082116-14-0

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH July 5, 2008.

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

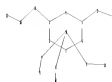
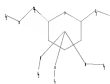
=> s ll

L1 NOT FOUND

The L-number entered has not been defined in this session, or it
has been deleted. To see the L-numbers currently defined in this
session, enter DISPLAY HISTORY at an arrow prompt (=>).

=>

Uploading C:\Program Files\STNEXP\Queries\10524048generic.str



```

chain nodes :
7  8  9 10 12 17 18 20 21 23 24
ring nodes :
1  2  3  4  5  6
chain bonds :
3-10  5-12  7-23  8-18  9-17 10-20 12-24 20-21
ring bonds :
1-2  1-6  2-3  3-4  4-5  5-6
exact/norm bonds :
1-2  1-6  2-3  3-4  4-5  5-6  5-12  7-23  8-18  9-17 12-24 20-21
exact bonds :
3-10 10-20

```

G1:O,S

G2:C,H

G3:C,S,P

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS

12:CLASS 13:CLASS 14:CLASS 15:CLASS 17:CLASS 18:CLASS 20:CLASS 21:CLASS
23:CLASS 24:CLASS

L1 STRUCTURE UPLOADED

=> s l1

SAMPLE SEARCH INITIATED 09:30:16 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 16061 TO ITERATE

12.5% PROCESSED 2000 ITERATIONS 50 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 313629 TO 328811
PROJECTED ANSWERS: 13600 TO 16914

L2 50 SEA SSS SAM L1

=> s l1 sss full

FULL SEARCH INITIATED 09:30:53 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 323752 TO ITERATE

100.0% PROCESSED 323752 ITERATIONS 15948 ANSWERS
SEARCH TIME: 00.00.02

L3 15948 SEA SSS FUL L1

=> file hcaplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	179.28	179.49

FILE 'HCAPLUS' ENTERED AT 09:30:58 ON 10 DEC 2008

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FILE COVERS 1907 - 10 Dec 2008 VOL 149 ISS 24

FILE LAST UPDATED: 9 Dec 2008 (20081209/ED)

HCaplus now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2008.

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l3
L4 6873 L3

=> file registry	SINCE FILE	TOTAL
COST IN U.S. DOLLARS	ENTRY	SESSION
FULL ESTIMATED COST	2.69	182.18

FILE 'REGISTRY' ENTERED AT 09:31:10 ON 10 DEC 2008
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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STRUCTURE FILE UPDATES: 8 DEC 2008 HIGHEST RN 1082116-14-0
DICTIONARY FILE UPDATES: 8 DEC 2008 HIGHEST RN 1082116-14-0

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH July 5, 2008.

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stdoc/properties.html>

=> log hold	SINCE FILE	TOTAL
COST IN U.S. DOLLARS	ENTRY	SESSION
FULL ESTIMATED COST	0.46	182.64

SESSION WILL BE HELD FOR 120 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 09:31:12 ON 10 DEC 2008

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSPTAEXO1623

PASSWORD:

* * * * * RECONNECTED TO STN INTERNATIONAL * * * * *
SESSION RESUMED IN FILE 'REGISTRY' AT 09:31:59 ON 10 DEC 2008
FILE 'REGISTRY' ENTERED AT 09:31:59 ON 10 DEC 2008
COPYRIGHT (C) 2008 American Chemical Society (ACS)

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
----------------------	------------	-------

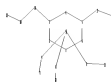
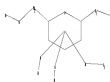
FULL ESTIMATED COST

ENTRY
0.46

SESSION
182.64

=>

Uploading C:\Program Files\STNEXP\Queries\10524048not2.str



```
chain nodes :  
7  8  9 10 12 17 18 20 21 23 24  
ring nodes :  
1  2  3 4 5 6  
chain bonds :  
3-10  5-12  7-23  8-18  9-17 10-20 12-24 20-21  
ring bonds :  
1-2  1-6  2-3  3-4  4-5  5-6  
exact/norm bonds :  
1-2  1-6  2-3  3-4  4-5  5-6  5-12  7-23 12-24  
exact bonds :  
3-10  8-18  9-17 10-20 20-21
```

G1:O,S

G2:C,H

G3:C,S,P

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
12:CLASS 13:CLASS 14:CLASS 15:CLASS 17:CLASS 18:CLASS 20:CLASS 21:CLASS
23:CLASS 24:CLASS

L5 STRUCTURE UPLOADED

=> s l5

SAMPLE SEARCH INITIATED 09:32:21 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 16061 TO ITERATE

12.5% PROCESSED 2000 ITERATIONS 45 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 313629 TO 328811
PROJECTED ANSWERS: 6087 TO 8367

L6 45 SEA SSS SAM L5

=> s l5 sss full

FULL SEARCH INITIATED 09:32:25 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 323752 TO ITERATE

100.0% PROCESSED 323752 ITERATIONS 6574 ANSWERS
SEARCH TIME: 00.00.02

L7 6574 SEA SSS FUL L5

=> s l3 not l5

L3 MAY NOT BE USED HERE

The L-number entered was not created by a STRUCTURE or SCREEN command.

=> s l3 not l7

L8 9374 L3 NOT L7

=> d his

(FILE 'HOME' ENTERED AT 09:29:04 ON 10 DEC 2008)

FILE 'REGISTRY' ENTERED AT 09:29:25 ON 10 DEC 2008

L1 STRUCTURE UPLOADED

L2 50 S L1

L3 15948 S L1 SSS FULL

FILE 'HCAPLUS' ENTERED AT 09:30:58 ON 10 DEC 2008

L4 6873 S L3

FILE 'REGISTRY' ENTERED AT 09:31:10 ON 10 DEC 2008

L5 STRUCTURE UPLOADED

L6 45 S L5
L7 6574 S L5 SSS FULL
L8 9374 S L3 NOT L7

=> log hold

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	178.82	361.00

SESSION WILL BE HELD FOR 120 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 09:32:54 ON 10 DEC 2008

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSPTAEXO1623

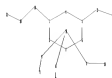
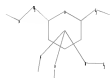
PASSWORD:

* * * * * RECONNECTED TO STN INTERNATIONAL * * * * *
SESSION RESUMED IN FILE 'REGISTRY' AT 09:33:41 ON 10 DEC 2008
FILE 'REGISTRY' ENTERED AT 09:33:41 ON 10 DEC 2008
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COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	178.82	361.00

=>

Uploading C:\Program Files\STNEXP\Queries\10524048not1.str



```

chain nodes :
7  8  9 10 12 17 18 20 21 23 24
ring nodes :
1  2  3  4  5  6
chain bonds :
3-10  5-12  7-23  8-18  9-17  10-20  12-24  20-21
ring bonds :
1-2  1-6  2-3  3-4  4-5  5-6
exact/norm bonds :
1-2  1-6  2-3  3-4  4-5  5-6  5-12  7-23  8-18  9-17  12-24  20-21
exact bonds :
3-10  10-20

```

G1:O,S

G2:C,H

G3:C,S,P

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
12:CLASS 13:CLASS 14:CLASS 15:CLASS 17:CLASS 18:CLASS 20:CLASS 21:CLASS
23:CLASS 24:CLASS

L9 STRUCTURE UPLOADED

=> s l9

SAMPLE SEARCH INITIATED 09:34:03 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 9642 TO ITERATE

20.7% PROCESSED 2000 ITERATIONS

50 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**

PROJECTED ITERATIONS: 186954 TO 198726

PROJECTED ANSWERS: 4414 TO 6384

L10 50 SEA SSS SAM L9

=> s l9 sss full

FULL SEARCH INITIATED 09:34:08 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 193254 TO ITERATE

100.0% PROCESSED 193254 ITERATIONS

5859 ANSWERS

SEARCH TIME: 00.00.01

L11 5859 SEA SSS FUL L9

=> d his

(FILE 'HOME' ENTERED AT 09:29:04 ON 10 DEC 2008)

FILE 'REGISTRY' ENTERED AT 09:29:25 ON 10 DEC 2008

L1 STRUCTURE UPLOADED

L2 50 S L1

L3 15948 S L1 SSS FULL

FILE 'HCAPLUS' ENTERED AT 09:30:58 ON 10 DEC 2008

L4 6873 S L3

FILE 'REGISTRY' ENTERED AT 09:31:10 ON 10 DEC 2008

L5 STRUCTURE UPLOADED

L6 45 S L5

L7 6574 S L5 SSS FULL

L8 9374 S L3 NOT L7

L9 STRUCTURE UPLOADED

L10 50 S L9

L11 5859 S L9 SSS FULL

=> s l8 not l11

L12 3518 L8 NOT L11

=> file hcaplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

	ENTRY	SESSION
FULL ESTIMATED COST	357.18	539.36

FILE 'HCAPLUS' ENTERED AT 09:34:25 ON 10 DEC 2008
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FILE COVERS 1907 - 10 Dec 2008 VOL 149 ISS 24
 FILE LAST UPDATED: 9 Dec 2008 (20081209/ED)

HCAplus now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2008.

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l12
 L13 1452 L12

=> s l13/prep
 FIELD CODES CANNOT BE CHANGED HERE
 You may have tried to apply a field code to a term that already has a field code. You can only add a field code to a term that has no field code appended to it.

=> s l12/prep
 1452 L12
 4682994 PREP/RL
 L14 1009 L12/PREP
 (L12 (L) PREP/RL)

=> file registry		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	2.69	542.05

FILE 'REGISTRY' ENTERED AT 09:34:50 ON 10 DEC 2008
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 DICTIONARY FILE UPDATES: 8 DEC 2008 HIGHEST RN 1082116-14-0

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH July 5, 2008.

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=> d his

(FILE 'HOME' ENTERED AT 09:29:04 ON 10 DEC 2008)

FILE 'REGISTRY' ENTERED AT 09:29:25 ON 10 DEC 2008

L1 STRUCTURE UPLOADED
L2 50 S L1
L3 15948 S L1 SSS FULL

FILE 'HCAPLUS' ENTERED AT 09:30:58 ON 10 DEC 2008

L4 6873 S L3

FILE 'REGISTRY' ENTERED AT 09:31:10 ON 10 DEC 2008

L5 STRUCTURE UPLOADED
L6 45 S L5
L7 6574 S L5 SSS FULL
L8 9374 S L3 NOT L7
L9 STRUCTURE UPLOADED
L10 50 S L9
L11 5859 S L9 SSS FULL
L12 3518 S L8 NOT L11

FILE 'HCAPLUS' ENTERED AT 09:34:25 ON 10 DEC 2008

L13 1452 S L12
L14 1009 S L12/PREP

FILE 'REGISTRY' ENTERED AT 09:34:50 ON 10 DEC 2008

=> log hold

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.46	542.51

SESSION WILL BE HELD FOR 120 MINUTES

STN INTERNATIONAL SESSION SUSPENDED AT 09:34:56 ON 10 DEC 2008

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSPTAEXO1623

PASSWORD:

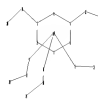
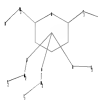
* * * * * RECONNECTED TO STN INTERNATIONAL * * * * *

SESSION RESUMED IN FILE 'REGISTRY' AT 09:38:09 ON 10 DEC 2008
 FILE 'REGISTRY' ENTERED AT 09:38:09 ON 10 DEC 2008
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COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	0.46	542.51

=>

Uploading C:\Program Files\STNEXP\Queries\10524048not3.str



```

chain nodes :
7  8  9 10 12 17 18 20 22 23 24 25
ring nodes :
1  2  3  4  5  6
chain bonds :
3-10  5-12  7-22  8-18  9-17 10-20 12-23 17-24 18-25
ring bonds :
1-2  1-6  2-3  3-4  4-5  5-6
exact/norm bonds :
1-2  1-6  2-3  3-4  4-5  5-6  5-12  7-22 12-23 17-24 18-25
  
```

exact bonds :
3-10 8-18 9-17 10-20

G1:O,S

G2:H,Ph

G3:C,S,P

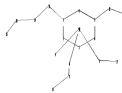
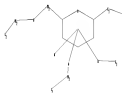
Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
12:CLASS 13:CLASS 14:CLASS 15:CLASS 17:CLASS 18:CLASS 20:CLASS 22:CLASS
23:CLASS 24:CLASS
25:CLASS

L15 STRUCTURE UPLOADED

=>

Uploading C:\Program Files\STNEXP\Queries\10524048not4.str



```

chain nodes :
7 8 9 10 12 17 19 21 22 23 24 25
ring nodes :
1 2 3 4 5 6
chain bonds :
3-10 5-12 7-21 8-17 10-19 12-22 17-23 19-24 24-25
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-12 7-21 12-22 17-23 24-25
exact bonds :
3-10 8-17 10-19 19-24

```

G1:O,S

G2:H,Ph

G3:C,S,P

```

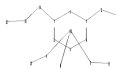
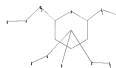
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
12:CLASS 13:CLASS 14:CLASS 15:CLASS 17:CLASS 19:CLASS 21:CLASS 22:CLASS
23:CLASS 24:CLASS
25:CLASS

```

L16 STRUCTURE UPLOADED

=>

Uploading C:\Program Files\STNEXP\Queries\10524048not5.str



```

chain nodes :
7  8  9 10 12 17 19 20 21 22
ring nodes :
1  2  3  4  5  6
chain bonds :
3-10  5-12  7-19  9-22 10-17 12-20 17-21
ring bonds :
1-2  1-6  2-3  3-4  4-5  5-6
exact/norm bonds :
1-2  1-6  2-3  3-4  4-5  5-6  5-12  7-19 12-20
exact bonds :
3-10  9-22 10-17 17-21

```

G1:O,S

G2:H,Ph

G3:C,S,P

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
12:CLASS 13:CLASS 14:CLASS 15:CLASS 17:CLASS 19:CLASS 20:CLASS 21:CLASS
22:CLASS

L17 STRUCTURE UPLOADED

=> d his

(FILE 'HOME' ENTERED AT 09:29:04 ON 10 DEC 2008)

FILE 'REGISTRY' ENTERED AT 09:29:25 ON 10 DEC 2008

L1 STRUCTURE UPLOADED

L2 50 S L1

L3 15948 S L1 SSS FULL

FILE 'HCAPLUS' ENTERED AT 09:30:58 ON 10 DEC 2008

L4 6873 S L3

FILE 'REGISTRY' ENTERED AT 09:31:10 ON 10 DEC 2008

L5 STRUCTURE UPLOADED

L6 45 S L5

L7 6574 S L5 SSS FULL

L8 9374 S L3 NOT L7

L9 STRUCTURE UPLOADED

L10 50 S L9

L11 5859 S L9 SSS FULL

L12 3518 S L8 NOT L11

FILE 'HCAPLUS' ENTERED AT 09:34:25 ON 10 DEC 2008

L13 1452 S L12

L14 1009 S L12/PREP

FILE 'REGISTRY' ENTERED AT 09:34:50 ON 10 DEC 2008

L15 STRUCTURE UPLOADED

L16 STRUCTURE UPLOADED

L17 STRUCTURE UPLOADED

=> s l15 sub=l12

ENTER SUBSET SEARCH SCOPE - SAMPLE, FULL, RANGE, OR (END):full

FULL SUBSET SEARCH INITIATED 09:39:25 FILE 'REGISTRY'

FULL SUBSET SCREEN SEARCH COMPLETED - 3518 TO ITERATE

100.0% PROCESSED 3518 ITERATIONS

135 ANSWERS

SEARCH TIME: 00.00.01

L18 135 SEA SUB=L12 SSS FUL L15

=> s l16 sub=l12

ENTER SUBSET SEARCH SCOPE - SAMPLE, FULL, RANGE, OR (END):full

FULL SUBSET SEARCH INITIATED 09:39:33 FILE 'REGISTRY'

FULL SUBSET SCREEN SEARCH COMPLETED - 2886 TO ITERATE

100.0% PROCESSED 2886 ITERATIONS

818 ANSWERS

SEARCH TIME: 00.00.01

L19 818 SEA SUB=L12 SSS FUL L16

=> s l17 sub=l12

ENTER SUBSET SEARCH SCOPE - SAMPLE, FULL, RANGE, OR (END):full
FULL SUBSET SEARCH INITIATED 09:39:43 FILE 'REGISTRY'
FULL SUBSET SCREEN SEARCH COMPLETED - 3518 TO ITERATE

100.0% PROCESSED 3518 ITERATIONS 1352 ANSWERS
SEARCH TIME: 00.00.01

L20 1352 SEA SUB=L12 SSS FUL L17

=> s l12 not l18
L21 3383 L12 NOT L18

=> s l21 not l19
L22 2567 L21 NOT L19

=> s l22 not l20
L23 1221 L22 NOT L20

=> file hcaplus	SINCE FILE	TOTAL
COST IN U.S. DOLLARS	ENTRY	SESSION
FULL ESTIMATED COST	128.14	670.19

FILE 'HCAPLUS' ENTERED AT 09:40:15 ON 10 DEC 2008
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FILE COVERS 1907 - 10 Dec 2008 VOL 149 ISS 24
FILE LAST UPDATED: 9 Dec 2008 (20081209/ED)

HCAplus now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2008.

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l23
L24 740 L23

=> s l23/prep
740 L23
4682994 PREP/RL
L25 561 L23/PREP
(L23 (L) PREP/RL)

=> file stnguide	SINCE FILE	TOTAL
COST IN U.S. DOLLARS		

	ENTRY	SESSION
FULL ESTIMATED COST	2.69	672.88

FILE 'STNGUIDE' ENTERED AT 09:40:30 ON 10 DEC 2008
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FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: Dec 5, 2008 (20081205/UP).

	SINCE FILE	TOTAL
	ENTRY	SESSION
=> file registry		
COST IN U.S. DOLLARS		
FULL ESTIMATED COST	0.54	673.42

FILE 'REGISTRY' ENTERED AT 09:45:51 ON 10 DEC 2008
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Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES: 8 DEC 2008 HIGHEST RN 1082116-14-0
DICTIONARY FILE UPDATES: 8 DEC 2008 HIGHEST RN 1082116-14-0

New CAS Information Use Policies, enter HELP USAGETERMS for details.

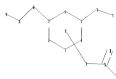
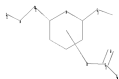
TSCA INFORMATION NOW CURRENT THROUGH July 5, 2008.

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=>
Uploading C:\Program Files\STNEXP\Queries\10524048narrow.str



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chain nodes :
7  8  10  13  14  16  17  18  20
ring nodes :
1  2  3  4  5  6
chain bonds :
3-8  5-10  7-16  8-13  10-17  13-14  16-18  16-20
ring bonds :
1-2  1-6  2-3  3-4  4-5  5-6
exact/norm bonds :
1-2  1-6  2-3  3-4  4-5  5-6  5-10  7-16  10-17  13-14  16-18  16-20
exact bonds :
3-8  8-13

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G1:O,S

G2:C,H

G3:C,S,P

G4:C,N

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 10:CLASS 11:CLASS
13:CLASS 14:CLASS 16:CLASS 17:CLASS 18:CLASS 20:CLASS

L26 STRUCTURE UPLOADED

=> s 126 sub=123

COMBINATION OF STRUCTURE AND TEXT TERMS NOT VALID

The query entered contains both search terms created by
structure-building or screen commands and text search terms. L#s
created via the STRUCTURE or SCREEN commands must be searched in the
structures files separately from text terms or profiles. The L#
answer sets from structure searches can be used in crossover searches
and can be combined with text terms.

=> s 126 sub=123

ENTER SUBSET SEARCH SCOPE - SAMPLE, FULL, RANGE, OR (END):full

FULL SUBSET SEARCH INITIATED 09:46:20 FILE 'REGISTRY'

FULL SUBSET SCREEN SEARCH COMPLETED - 1201 TO ITERATE

100.0% PROCESSED 1201 ITERATIONS

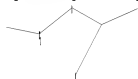
1024 ANSWERS

SEARCH TIME: 00.00.01

L27 1024 SEA SUB=L23 SSS FUL L26

=>

Uploading C:\Program Files\STNEXP\Queries\10524048groupy.str



chain nodes :

4 5 6 7 8 9

chain bonds :

4-5 4-9 5-6 6-7 6-8

exact/norm bonds :

5-6

exact bonds :

4-5 4-9 6-7 6-8

G1:O,S

G2:H,Ph

G3:C,S,P

Match level :

4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS

L28 STRUCTURE UPLOADED

=> s 128 sub=127

ENTER SUBSET SEARCH SCOPE - SAMPLE, FULL, RANGE, OR (END):full

FULL SUBSET SEARCH INITIATED 09:46:51 FILE 'REGISTRY'

FULL SUBSET SCREEN SEARCH COMPLETED - 909 TO ITERATE

100.0% PROCESSED 909 ITERATIONS

12 ANSWERS

SEARCH TIME: 00.00.01

L29 12 SEA SUB=L27 SSS FUL L28

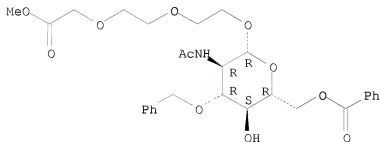
=> d 129 scan

L29 12 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN

IN Acetic acid, [2-[2-[[2-(acetylamino)-6-O-benzoyl-2-deoxy-3-O-(phenylmethyl)-β-D-glucopyranosyl]oxy]ethoxy]ethoxy]-, methyl ester (9CI)

MF C29 H37 N O11

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

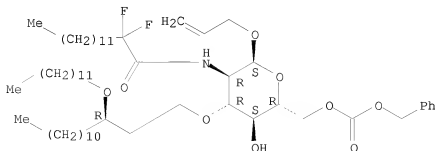
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):3

L29 12 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN

IN α-D-Glucopyranoside, 2-propenyl 2-deoxy-2-[[2,2-difluoro-1-oxotetradecyl]amino]-3-O-[(3R)-3-(dodecyloxy)tetradecyl]-, 6-(phenylmethyl carbonate) (9CI)

MF C57 H99 F2 N O9

Absolute stereochemistry.



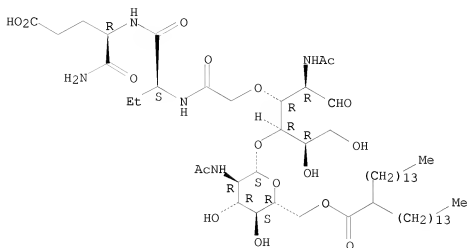
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L29 12 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN

IN Pentanoic acid, 4-[[[(2S)-2-[[[N-acetyl-4-O-[2-(acetylamino)-2-deoxy-6-O-(1-oxo-2-tetradecylhexadecyl)- β -D-glucopyranosyl]normuramoyl]amino]-1-oxobutyl]amino]-5-amino-5-oxo-, (4R)- (9CI)

MF C57 H103 N5 O17

Absolute stereochemistry.



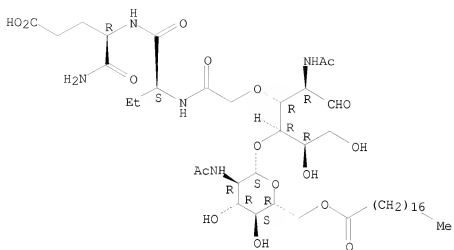
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L29 12 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN

IN Pentanoic acid, 4-[[[(2S)-2-[[[N-acetyl-4-O-[2-(acetylamino)-2-deoxy-6-O-(1-oxooctadecyl)- β -D-glucopyranosyl]normuramoyl]amino]-1-oxobutyl]amino]-5-amino-5-oxo-, (4R)- (9CI)

MF C45 H79 N5 O17

Absolute stereochemistry.



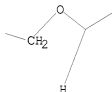
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> d l28

L28 HAS NO ANSWERS

L28 STR



G1 O, S

G2 H, Ph

G3 C, S, P

Structure attributes must be viewed using STN Express query preparation.

=>

Uploading C:\Program Files\STNEXP\Queries\10524048groupy2.str



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chain nodes :
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chain bonds :
1-2 1-6 2-3 3-4 3-5
exact/norm bonds :
1-6 2-3
exact bonds :
1-2 3-4 3-5

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G1:C,H

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Match level :
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS

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L30 STRUCTURE UPLOADED

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=> s 130 sub=127
ENTER SUBSET SEARCH SCOPE - SAMPLE, FULL, RANGE, OR (END):full
FULL SUBSET SEARCH INITIATED 09:48:54 FILE 'REGISTRY'
FULL SUBSET SCREEN SEARCH COMPLETED - 1024 TO ITERATE

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100.0% PROCESSED 1024 ITERATIONS
SEARCH TIME: 00.00.01

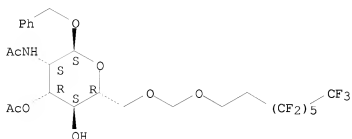
110 ANSWERS

L31 110 SEA SUB=L27 SSS FUL L30

=> d 131 scan

L31 110 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN α -D-Mannopyranoside, phenylmethyl
2-(acetylamino)-2-deoxy-6-O-[[[3,3,4,4,5,5,6,6,7,7,8,8,8-
tridecafluorooctyl]oxy]methyl]-, 3-acetate
MF C26 H28 F13 N O8

Absolute stereochemistry.

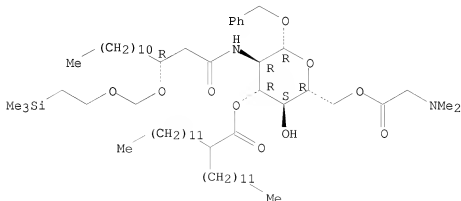


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):2

L31 110 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN Glycine, N,N-dimethyl-, 6-ester with phenylmethyl
2-deoxy-2-[[1-oxo-3-[[2-(trimethylsilyl)ethoxy]methoxy]tetradecyl]amino]-
 β -D-glucopyranoside 3-(2-dodecyltetradecanoate), (R)- (9CI)
MF C63 H116 N2 O10 Si

Absolute stereochemistry.



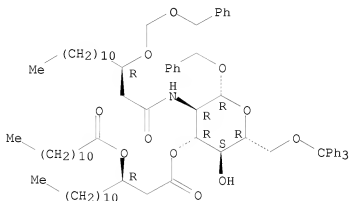
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L31 110 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN

IN β -D-Glucopyranoside, phenylmethyl
2-deoxy-2-[[1-oxo-3-[(phenylmethoxy)methoxy]tetradecylamino]-6-O-
(triphenylmethyl)-, 3-[3-[(1-oxododecyl)oxy]tetradecanoate], [2(R),3(R)]-
(9CI)

MF C80 H115 N O11

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> file hcaplus
COST IN U.S. DOLLARS
FULL ESTIMATED COST

SINCE FILE	TOTAL
ENTRY	SESSION
129.06	802.48

FILE 'HCAPLUS' ENTERED AT 09:49:12 ON 10 DEC 2008

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FILE COVERS 1907 - 10 Dec 2008 VOL 149 ISS 24
FILE LAST UPDATED: 9 Dec 2008 (20081209/ED)

HCAPLUS now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2008.

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This file contains CAS Registry Numbers for easy and accurate substance identification.

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=> s 131
L32          52 L31

=> s 132 and (PY<2003 or AY<2003 or PRY<2003)
22961967 PY<2003
4500767 AY<2003
3969216 PRY<2003
L33          42 L32 AND (PY<2003 OR AY<2003 OR PRY<2003)

=> d 133 1-42 ti abs bi bhitstr
'BI' IS NOT A VALID FORMAT FOR FILE 'HCAPLUS'
'BHITSTR' IS NOT A VALID FORMAT FOR FILE 'HCAPLUS'
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The following are valid formats:

```
ABS ----- GI and AB
ALL ----- BIB, AB, IND, RE
APPS ----- AI, PRAI
BIB ----- AN, plus Bibliographic Data and PI table (default)
CAN ----- List of CA abstract numbers without answer numbers
CBIB ----- AN, plus Compressed Bibliographic Data
CLASS ----- IPC, NCL, ECLA, FTERM
DALL ----- ALL, delimited (end of each field identified)
DMAX ----- MAX, delimited for post-processing
FAM ----- AN, PI and PRAI in table, plus Patent Family data
FBIB ----- AN, BIB, plus Patent FAM
IND ----- Indexing data
IPC ----- International Patent Classifications
MAX ----- ALL, plus Patent FAM, RE
PATS ----- PI, SO
SAM ----- CC, SX, TI, ST, IT
SCAN ----- CC, SX, TI, ST, IT (random display, no answer numbers;
SCAN must be entered on the same line as the DISPLAY,
e.g., D SCAN or DISPLAY SCAN)
STD ----- BIB, CLASS

IABS ----- ABS, indented with text labels
IALL ----- ALL, indented with text labels
IBIB ----- BIB, indented with text labels
IMAX ----- MAX, indented with text labels
ISTD ----- STD, indented with text labels

OBIB ----- AN, plus Bibliographic Data (original)
OIBIB ----- OBIB, indented with text labels

SBIB ----- BIB, no citations
SIBIB ----- IBIB, no citations

HIT ----- Fields containing hit terms
HITIND ----- IC, ICA, ICI, NCL, CC and index field (ST and IT)
containing hit terms
HITRN ----- HIT RN and its text modification
HITSTR ----- HIT RN, its text modification, its CA index name, and
```

its structure diagram
HITSEQ ----- HIT RN, its text modification, its CA index name, its
structure diagram, plus NTE and SEQ fields
FHITSTR ----- First HIT RN, its text modification, its CA index name, and
its structure diagram
FHITSEQ ----- First HIT RN, its text modification, its CA index name, its
structure diagram, plus NTE and SEQ fields
KWIC ----- Hit term plus 20 words on either side
OCC ----- Number of occurrence of hit term and field in which it occurs

To display a particular field or fields, enter the display field
codes. For a list of the display field codes, enter HELP DFIELDS at
an arrow prompt (=>). Examples of formats include: TI; TI,AU; BIB,ST;
TI,IND; TI,SO. You may specify the format fields in any order and the
information will be displayed in the same order as the format
specification.

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FHITSTR, HITSEQ, FHITSEQ, KWIC, and OCC) may be used with DISPLAY ACC
to view a specified Accession Number.
ENTER DISPLAY FORMAT (BIB):ti abs bib hitstr

L33 ANSWER 1 OF 42 HCAPLUS COPYRIGHT 2008 ACS on STN
TI Preparation of glycosides of N-acetyl-6-O-[2,2-bis(hydroxymethyl)-3-
hydroxypropyl]-D-glucosamine for use in the treatment of brain tumors
AB The invention describes the preparation of title glycosides (aglycon R1 =
C8-C16 alkyl) from N-acetyl-D-glucosamine. The procedure involves
glycosidation (e.g., with octanol), reaction of the 4,5-dibenzyl-protected
derivative with 9-(4-methoxyphenyl)-2,4,8,10-tetraoxa-3-thiaspiro[5.5]undecane
3,3-dioxide (prepared from pentaerythritol, anisaldehyde, and
1,1'-sulfonyldiimidazole), and deprotection. Octyl
2-acetamido-6-O-[2,2-bis(hydroxymethyl)-3-hydroxypropyl]- α -D-
glucosamine showed IC50 = 43 \pm 14 μ M for inhibition of human glioma
cultures.
AN 2001:780924 HCAPLUS <<LOGINID:20081210>>
DN 135:331634
TI Preparation of glycosides of N-acetyl-6-O-[2,2-bis(hydroxymethyl)-3-
hydroxypropyl]-D-glucosamine for use in the treatment of brain tumors
IN Bernabe Pajares, Manuel; Fernandez-Mayoralas, Alvarez Alfonso; Nieto
Sampedro, Manuel; Vaquero Crespo, Jesus; Zurita Castillo, Mercedes
PA Consejo Superior De Investigaciones Cientificas, Spain; Hospital
Universitario Clinica Puerta De Hierro
SO PCT Int. Appl., 18 pp.
CODEN: PIXXD2
DT Patent
LA Spanish
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001079243	A1	20011025	WO 2001-ES138	20010406 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,				
CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR,				
HR, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT,				
LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU,				
SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN,				
YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,				
DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,				
BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
ES 2164013	A1	20020201	ES 2000-982	20000414 <--
ES 2164013	B1	20030616		

PRAI ES 2000-982 A 20000414 <--

OS CASREACT 135:331634; MARPAT 135:331634

IT 368870-53-5P

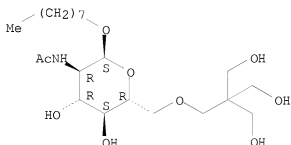
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)

(preparation of glycosides of acetyl[bis(hydroxymethyl)hydroxypropyl]-D-glucosamine for treatment of brain tumors)

RN 368870-53-5 HCAPLUS

CN α -D-Glucopyranoside, octyl 2-(acetylamino)-2-deoxy-6-O-[3-hydroxy-2,2-bis(hydroxymethyl)propyl]- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



IT 368870-57-9P

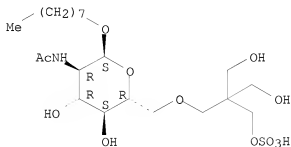
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of glycosides of acetyl[bis(hydroxymethyl)hydroxypropyl]-D-glucosamine for treatment of brain tumors)

RN 368870-57-9 HCAPLUS

CN α -D-Glucopyranoside, octyl 2-(acetylamino)-6-O-[2,2-bis(hydroxymethyl)-3-(sulfooxy)propyl]-2-deoxy-, monosodium salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.

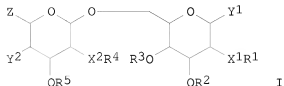


● Na

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L33 ANSWER 2 OF 42 HCAPLUS COPYRIGHT 2008 ACS on STN

TI Preparation of oligosaccharide lipid-A analogs as antitumor and immunostimulating agents



AB New synthetic sugar Lipid-A analogs I wherein at least one of R1-R5 is selected from RCONHCH[R'NHCO]CH2CO-, RCH[X](CH2)mAOCHR'(CH2)nB-, RAOCHR'(CH2)mBOCHR"(CH2)nL-, where the remaining R1-R5 AR IDP H, R, COR, RCONHCH[R'NHCO]CH2CO-, RCH[X](CH2)mAOCHR'(CH2)nB-, RAOCHR'(CH2)mBOCHR"(CH2)nL-, RCH(X)(CH2)mA-, RAOCHR'(CH2)mB-, where each R, R', R" is independently H, alkyl, A, B and L are independently selected from the group consisting of -CH-, -C(=O)- and -C(=S) groups; each X is independently selected from the group consisting of -OH, -SH, -NH, and-halogen; m and n are independently selected from the range of integers between 0 and 10 inclusive, X1 and X are -O- or -NH-, Y1 and Y2 are independently selected from the group consisting of -OH, -OP(O)(OH), -COOH, -OSOH, -CH(COOH) and -OP(O)(OH)(OCHCHNH), Z is H, -CHE, or -CHMG, where E is hydrogen, halogen, OH, NH, OSOH, SOH, P(O)(OH) or OP(O)(OH); M is -O-, -S-, -OC(=O), -SC(=O), -OC(=S)-, or -NHC(=O); G is -hydrogen, or a substituted or unsubstituted, branched or linear, saturated or unsatd. C-2 aliphatic hydrocarbon. or a physiol. acceptable salt thereof. Liposome formulations containing totally synthetic components such as synthetic Lipid-A and synthetic lipopeptide derived from tumor-associated MUC1 mucin are described along with their therapeutic utility. Comparative test results of immunostimulating properties and toxicity of Lipid-A analogs are included. Thus, 2-deoxy-4-O-phosphono-2-[(3S)-3-tetradecanamido-4-nonylamino-4-oxo-butanamido]-3-O-tetradecanoyl-D-glucopyranose was prepared and tested in mice as antitumor and immunostimulating agent (CPM = m22). 2001:380597 HCAPLUS <<LOGINID:20081210>>

AN 134:367137

TI Preparation of oligosaccharide lipid-A analogs as antitumor and immunostimulating agents

IN Jiang, Zi-Hua; Bach, Mimi; Yalamati, Damayanthi; Koganty, Rao; Longenecker, Michael

PA Biomira, Inc., Can.

SO PCT Int. Appl., 155 pp.

CODEN: P1XXD2

DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2001036433	A2	20010525	WO 2000-US31281	20001115 <--
	WO 2001036433	A3	20020510		
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DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,
 BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

CA 2396744	A1	20010525	CA 2000-2396744	20001115 <--
AU 2001017647	A	20010530	AU 2001-17647	20001115 <--
AU 780577	B2	20050407		
EP 1232168	A2	20020821	EP 2000-980380	20001115 <--

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
 IE, SI, LT, LV, FI, RO, MK, CY, AL, TR

JP 2003514824	T	20030422	JP 2001-538922	20001115 <--
PRAI US 1999-164928P	P	19991115	<--	
WO 2000-US31281	W	20001115	<--	

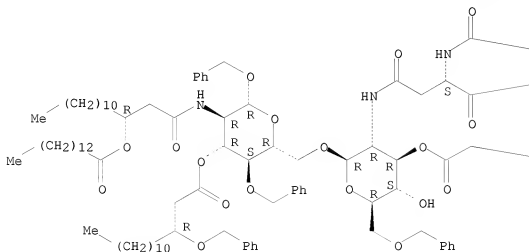
OS MARPAT 134:367137
 IT 339317-13-4P

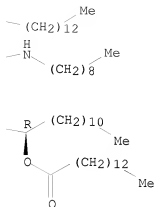
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation of oligosaccharide lipid A analogs as antitumor and
 immunostimulating agents)

RN 339317-13-4 HCAPLUS
 CN β -D-Glucopyranoside, phenylmethyl
 2-deoxy-6-O-[2-deoxy-2-[[[(3S)-4-(nonylamino)-1,4-dioxo-3-[(1-oxotetradecyl)amino]butyl]amino]-3-O-[(3R)-1-oxo-3-[(1-oxotetradecyl)oxy]tetradecyl]-6-O-(phenylmethyl)- β -D-glucopyranosyl]-2-[[[(3R)-1-oxo-3-[(1-oxotetradecyl)oxy]tetradecyl]amino]-4-O-(phenylmethyl)-, 3-[(3R)-3-(phenylmethoxy)tetradecanoate] (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

PAGE 1-A

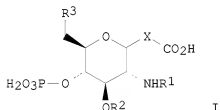




L33 ANSWER 3 OF 42 HCAPLUS COPYRIGHT 2008 ACS on STN

TI Preparation of ether-type lipid GLA-60 analogues inhibiting the activation of macrophage

GI



I

AB The title compds. (I), esters of the same, or pharmacol. acceptable salts thereof, [wherein R1 is (un)substituted C1-20 alkanoyl, C3-20 alkenoyl, or C3-20 alkynoyl; R2 is C1-20 alkyl, C2-20 alkenyl, or C2-20 alkynyl; R3 is halogeno, hydroxyl, C1-6 alkoxy, C2-6 alkenyloxy, or C2-6 alkynyloxy; and X is a single bond or OCH2] are prepared. These compds., esters and salts exhibit an excellent macrophage-depressant effect and are useful as anti-inflammatory, antiautoimmune or antisepticemic agents. Thus, 2,6-anhydro-3-deoxy-3-(2,2-difluorotetradecanamido)-5-O-phosphono-4-O-[(R)-3-(dodecyloxy)tetradecyl]-7-O-methyl-D-glycero-D-ido-heptonic acid in THF was hydrogenolyzed over platinum oxide under hydrogen atmospheric

at room temperature for 18 h to give 2,6-anhydro-3-deoxy-3-(2,2-difluorotetradecanamido)-5-O-phosphono-4-O-[(R)-3-(dodecyloxy)tetradecyl]-7-O-methyl-D-glycero-D-ido-heptonic acid, which showed IC50 of 1.5 nM for inhibiting the lipopolysaccharide (LPS)-stimulated production of TNF α in TPA-treated human monocyte U937 cells.

AN 2001:338537 HCAPLUS <<LOGINID:20081210>>

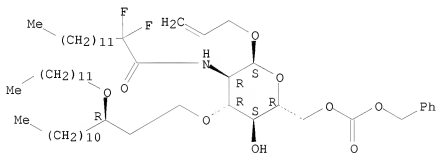
DN 134:353476

TI Preparation of ether-type lipid GLA-60 analogues inhibiting the activation

of macrophage
 IN Watanabe, Yukiko; Miura, Kumiko; Nakamura, Tsuyoshi; Shiozaki, Masao
 PA Sankyo Co., Ltd., Japan
 SO PCT Int. Appl., 197 pp.
 CODEN: PIXXD2
 DT Patent
 LA Japanese
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2001032667	A1	20010510	WO 2000-JP7759	20001102 <--
	W: AU, BR, CA, CN, CZ, HU, ID, IL, IN, KR, MX, NO, NZ, PL, RU, US, ZA				
	RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR				
	JP 2001270895	A	20011002	JP 2000-335543	20001102 <--
PRAI	JP 1999-314133	A	19991104	<--	
	JP 2000-4254	A	20000113	<--	
OS	MARPAT 134:353476				
IT	338951-92-1P				
	RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)				
	(preparation of ether-type lipid GLA-60 analogs inhibiting activation of macrophage as anti-inflammatory, antiautoimmune, or antisepticemic agents)				
RN	338951-92-1 HCAPLUS				
CN	α -D-Glucopyranoside, 2-propenyl 2-deoxy-2-[(2,2-difluoro-1-oxotetradecyl)amino]-3-O-[(3R)-3-(dodecyloxy)tetradecyl]-, 6-(phenylmethyl carbonate) (9CI) (CA INDEX NAME)				

Absolute stereochemistry.



RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L33 ANSWER 4 OF 42 HCAPLUS COPYRIGHT 2008 ACS on STN
 TI Approach to transition state analog of glycosyltransferase reaction.
 Design and synthesis of selective inhibitor of β -1,4-galactosyltransferase
 AB A review with 23 refs. In order to create specific inhibitors against glycosyltransferases, tethering glycosyl donor to acceptor was planned. Mono-O-methylated UDP-Gal and related analogs were synthesized, and their behaviors toward β -1,4-galactosyltransferase were examined. The allowance for the O-methylation of Gal moiety was decreased in the following order: 2-, 3-, 4-, and 6-positions and it was suggested that the modification at the 2-position does not affect the affinity but retards the reaction rate by preventing the conformational change to the

transition state, which develops so-called dynamic binding. Modification of the glycosyl acceptor (GlcNAc) moiety showed the tethering probability in the 3'- and 6'-positions. Bisubstrate tricomponent analogs linked through 2,6'-methylene and 2,6'-ethylene groups were synthesized and found to be potent inhibitors against bovine GlcNAc:β-1,4-galactosyltransferase, with K_i values of 1.35 and 1.95 μM, resp., for the acceptor.

AN 1997:264954 HCAPLUS <<LOGINID:20081210>>

DN 127:5238

OREF 127:1193a,1196a

TI Approach to transition state analog of glycosyltransferase reaction. Design and synthesis of selective inhibitor of β-1,4-galactosyltransferase

AU Hashimoto, Hironobu; Kajihara, Yasuhiro

CS Dep. Life Sci., Tokyo Inst. Technol., Yokohama, 226, Japan

SO Yuki Gosei Kagaku Kyokaishi (1997), 55(4), 325-333

CODEN: YGKKAE; ISSN: 0037-9980

PB Yuki Gosei Kagaku Kyokai

DT Journal; General Review

LA Japanese

IT 190248-89-6P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(design and preparation of selective inhibitor of β-1,4-galactosyltransferase)

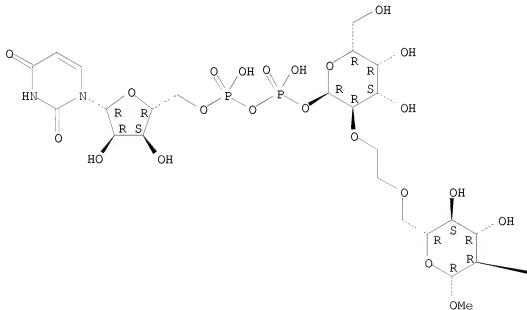
RN 190248-89-6 HCAPLUS

CN Uridine 5'-(trihydrogen diphosphate),

P'-[2-O-[2-[2-(acetylamino)-2-deoxy-1-O-methyl-β-D-glucopyranos-6-O-yl]ethyl]-α-D-galactopyranosyl] ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

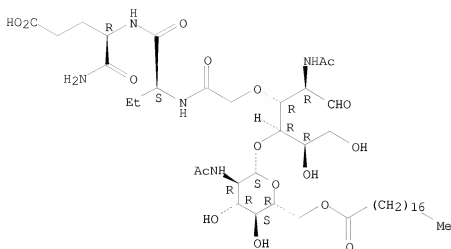
PAGE 1-A



NHAC

L33 ANSWER 5 OF 42 HCAPLUS COPYRIGHT 2008 ACS on STN
 TI Immunomodulatory and radioprotective activities of synthetic analogs of
 the disaccharide-dipeptide subunit of peptidoglycan
 AB Glycopeptides derived from bacterial cell wall peptidoglycans possess
 marked immunostimulatory properties. The min. adjuvant-active structure
 of peptidoglycan is MDP, however, some compds. with a prolonged sugar
 chain derived from the basal repeating disaccharide-dipeptide unit (GMDP)
 are more potent and less toxic. Here, the authors present several biol.
 activities of a totally synthetic GMDP analog modified both in the sugar
 and in the peptide part, and its lipophilic derivs.
 AN 1996:639657 HCAPLUS <<LOGINID::20081210>>
 DN 126:139608
 OREF 126:26823a,26826a
 TI Immunomodulatory and radioprotective activities of synthetic analogs of
 the disaccharide-dipeptide subunit of peptidoglycan
 AU Hribalova, V.; Vacek, A.; Toman, M.; Horavova, P.; Ledvina, M.; Jezek, J.
 CS National Institute Public Health, Prague, CZ-100 42, Czech Rep.
 SO Peptides 1994, Proceedings of the European Peptide Symposium, 23rd, Braga,
 Port., Sept. 4-10, 1994 (1995), Meeting Date 1994, 847-848.
 Editor(s): Maia, Hernani L. S. Publisher: ESCOM, Leiden, Neth.
 CODEN: 63MBAO
 DT Conference
 LA English
 IT 155780-14-6
 RL: ADV (Adverse effect, including toxicity); BIOL (Biological study)
 (immunostimulatory and radioprotective activities of muramyl dipeptide
 analogs)
 RN 155780-14-6 HCAPLUS
 CN Pentanoic acid, 4-[[[(2S)-2-[[[N-acetyl-4-O-[2-(acetilamino)-2-deoxy-6-O-(1-
 oxooctadecyl)-β-D-glucopyranosyl]normuramoyl]amino]-1-oxobutyl]amino]-
 5-amino-5-oxo-, (4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



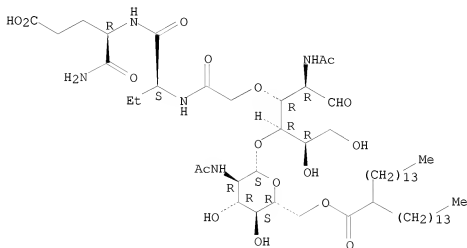
IT 155780-15-7

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(immunostimulatory and radioprotective activities of muramyl dipeptide analogs)

RN 155780-15-7 HCAPLUS

CN Pentanoic acid, 4-[[[(2S)-2-[[N-acetyl-4-O-[2-(acetyl-amino)-2-deoxy-6-O-(1-oxo-2-tetradecylhexadecyl)-β-D-glucopyranosyl]normuramoyl]amino]-1-oxobutyl]amino]-5-amino-5-oxo-, (4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L33 ANSWER 6 OF 42 HCAPLUS COPYRIGHT 2008 ACS on STN

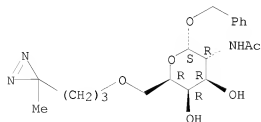
TI Synthesis of O-glycan core 3: characterization of UDP-GlcNAc:GalNAc-R β3-N-acetyl-glucosaminyltransferase activity from colonic mucosal tissues and lack of the activity in human cancer cell lines

AB UDP-GlcNAc:GalNAc-R β3-GlcNAc-transferase (core 3 β3-GlcNAc-T, where GlcNAc is N-acetyl-D-glucosamine, GalNAc is N-acetyl-D-galactosamine and T is transferase) is expressed in a tissue-specific fashion and is high in normal colonic tissue, but down regulated in colon cancer. To

further study the control of this enzyme, we examined the activity in pig, rat and human colonic tissues, and several human cancer cell lines. The enzyme was difficult to solubilize by detergents and was extremely unstable in the solubilized form. Using synthetic derivs. of the GalNAc-R substrate, we showed that the specificity of the enzyme in normal rat and human colonic mucosa requires all the substituents of the GalNAc-sugar ring of substrates for maximal activity. Core 3 β 3-GlcNAc-T was significantly influenced by the structure of the aglycon group. None of the inactive substrate derivs. could inhibit the activity. N-iodoacetamido-galactosamine- α -benzyl was a weak substrate and significantly inhibited the incorporation of GlcNAc into Gal-NAc- α -benzyl by human colonic homogenates. Surprisingly, none of the colonic cancer cell lines or any other cancer and leukemia cells examined exhibited detectable activity of the enzyme, although a number of other glycosyltransferase activities involved in O-glycan biosynthesis were active. Mixing expts. did not reveal an endogenous inhibitor in HL60 cells or an activator of core 3 β 3-GlcNAc-T in human colonic mucosa. Thus, the lack of core 3 β 3-GlcNAc-T activity in cancer cell lines may be due to cell transformation or cell culturing.

AN 1995:592627 HCAPLUS <<LOGINID::20081210>>
 DN 123:163928
 OREF 123:29091a,29094a
 TI Synthesis of O-glycan core 3: characterization of UDP-GlcNAc:GalNAc-R β 3-N-acetyl-glucosaminyltransferase activity from colonic mucosal tissues and lack of the activity in human cancer cell lines
 AU Vavasseur, Fabienne; Yang, Ji-Mao; Dole, Kiran; Paulsen, Hans; Brockhausen, Inka
 CS Dep. Biochemistry, Hospital Sick Children, Toronto, ON, Can.
 SO Glycobiology (1995), 5(3), 351-7
 CODEN: GLYCE3; ISSN: 0959-6658
 PB Oxford University Press
 DT Journal
 LA English
 IT 141019-97-8 142925-54-0 166907-10-4
 166907-11-5
 RL BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study); PROC (Process)
 (substrate; substrate specificity of UDP-GlcNAc:GalNAc-R β 3-N-acetyl-glucosaminyltransferase from colonic mucosa and lack of activity in human cancer cell lines)
 RN 141019-97-8 HCAPLUS
 CN α -D-Galactopyranoside, phenylmethyl
 2-(acetylamino)-2-deoxy-6-O-[3-(3-methyl-3H-diazirin-3-yl)propyl]- (CA INDEX NAME)

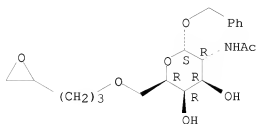
Absolute stereochemistry.



RN 142925-54-0 HCAPLUS
 CN α -D-Galactopyranoside, phenylmethyl

2-(acetylamino)-2-deoxy-6-O-(3-oxiranylpropyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

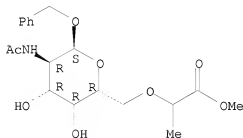


RN 166907-10-4 HCAPLUS

CN α-D-Galactopyranoside, phenylmethyl

2-(acetylamino)-2-deoxy-6-O-(2-methoxy-1-methyl-2-oxoethyl)- (CA INDEX NAME)

Absolute stereochemistry.

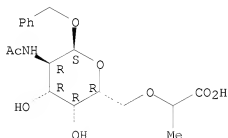


RN 166907-11-5 HCAPLUS

CN α-D-Galactopyranoside, phenylmethyl

2-(acetylamino)-6-O-(1-carboxyethyl)-2-deoxy- (CA INDEX NAME)

Absolute stereochemistry.



L33 ANSWER 7 OF 42 HCAPLUS COPYRIGHT 2008 ACS on STN

TI Fragmentation of lipophilic disaccharide analogs of muramyl dipeptide (MDP) in FAB mass spectrometry, a characterization of lipophilic substitution

AB Fast-atom-bombardment mass spectra of disaccharide analogs of muramyl

dipeptide are reported.

AN 1995:592524 HCAPLUS <<LOGINID::20081210>>

DN 123:257185

OREF 123:46015a,46018a

TI Fragmentation of lipophilic disaccharide analogs of muramyl dipeptide (MDP) in FAB mass spectrometry, a characterization of lipophilic substitution

AU Vaisar, Tomas; Ledvina, Miroslav; Jezek, Jan

CS Inst. Org. Chem. Biochem., Acad. Sci. Czech Republic, Prague, 166 10, Czech Rep.

SO Journal of Mass Spectrometry (1995), 30(5), 767-8

CODEN: JMSPFJ; ISSN: 1076-5174

PB Wiley

DT Journal

LA English

IT 155780-14-6 155780-15-7

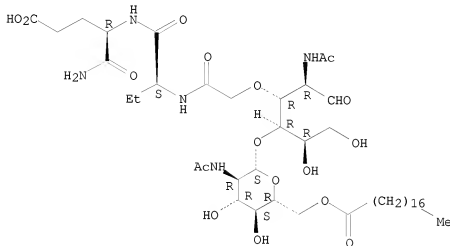
RL: PRP (Properties)

(fragmentation of lipophilic disaccharide analogs of muramyl dipeptide using fast-atom-bombardment mass spectrometry)

RN 155780-14-6 HCAPLUS

CN Pentanoic acid, 4-[[[(2S)-2-[[N-acetyl-4-O-[2-(acetyl-amino)-2-deoxy-6-O-(1-oxooctadecyl)-β-D-glucopyranosyl]normuramoyl]amino]-1-oxobutyl]amino]-5-amino-5-oxo-, (4R)- (9CI) (CA INDEX NAME)

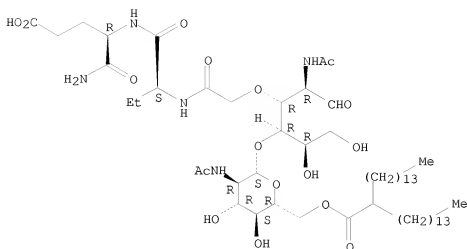
Absolute stereochemistry.



RN 155780-15-7 HCAPLUS

CN Pentanoic acid, 4-[[[(2S)-2-[[N-acetyl-4-O-[2-(acetyl-amino)-2-deoxy-6-O-(1-oxo-2-tetradecylhexadecyl)-β-D-glucopyranosyl]normuramoyl]amino]-1-oxobutyl]amino]-5-amino-5-oxo-, (4R)- (9CI) (CA INDEX NAME)

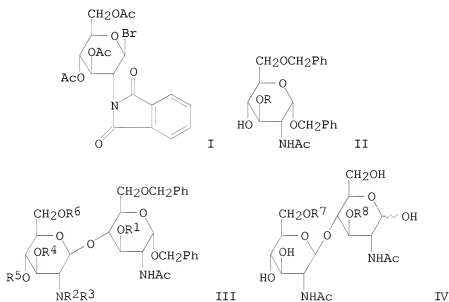
Absolute stereochemistry.



L33 ANSWER 8 OF 42 HCAPLUS COPYRIGHT 2008 ACS on STN

TI Synthesis of O-[2-acetamido-2-deoxy-6-O-stearoyl- and -6-O-(2-tetradecylhexadecanoyl)-β-D-glucopyranosyl]-(1 → 4)-N-acetyl normuramoyl-L-α-aminobutanoyl-D-isoglutamine, lipophilic disaccharide analogs of MDP

GI



AB Silver triflate-promoted condensation of

3,4,6-tri-O-acetyl-2-deoxy-2-phthalimido-β-D-glucopyranosyl bromide (I) with benzyl 2-acetamido-6-O-benzyl-2-deoxy-3-O-(methoxycarbonyl)methyl-α-D-glucopyranoside (II; R = CH₂CO₂Me) afforded the key compound, benzyl 2-acetamido-6-O-benzyl-2-deoxy-3-O-(methoxycarbonyl)methyl-4-O-(3,4,6-tri-O-acetyl-2-deoxy-2-phthalimido-β-D-glucopyranosyl)-α-D-glucopyranoside (II; R₁ = CH₂CO₂Me, R₂R₃ = 1,2-OCC₆H₄CO, R₄ - R₆ = Ac),

which after deprotection was transformed into acid II (R1 = CH₂CO₂H, R₂ = H, R₃ = Ac, R₅R₆ = CMe₂). Condensation of II (R1 = CH₂CO₂H, R₂ = H, R₃ = Ac, R₅R₆ = CMe₂) with the benzyl ester of L- α -aminobutanoyl-D-isoglutamine and deisopropylidenation of the product II [R1 = CH₂CO-L-Abu-D-isoGln(OCH₂Ph), R₂ = H, R₃ = Ac, R₄ = CH₂OCH₂Ph, R₅R₆ = CMe₂, Abu = EtCH(NH)CO] afforded the benzyl ester of N-(2-O-[benzyl 2-acetamido-4-O-(2-acetamido-3-O-benzoyloxymethyl-2-deoxy- β -D-glucopyranosyl)-6-O-benzyl-2,3-dideoxy- α -D-glucopyranosid-3-yl]glycoloyl)- α -aminobutanoyl-D-isoglutamine [II; R1 = CH₂CO-L-Abu-D-isoGln(OCH₂Ph), R₂ = R₅ = R₆ = H, R₃ = Ac, R₄ = CH₂OCH₂Ph]. Partial O-acylation of II [R1 = CH₂CO-L-Abu-D-isoGln(OCH₂Ph), R₂ = R₅ = R₆ = H, R₃ = Ac, R₄ = CH₂OCH₂Ph] and hydrogenolysis of protecting groups gave the 6-O-stearoyl- and 6-O-(2-tetradecylhexadecanoyl)-disaccharide-dipeptides IV [R₇ = stearoyl, 2-(tetradecyl)hexadecanoyl, R₈ = CH₂CO-L-Abu-D-isoGln], resp. Pyrogenicity and adjuvant activity in cell-mediated immunity are reported.

AN 1994:436053 HCAPLUS <<LOGINID:20081210>>

DN 121:36053

OREF 121:6683a,6686a

TI Synthesis of O-[2-acetamido-2-deoxy-6-O-stearoyl- and -6-O-(2-tetradecylhexadecanoyl)- β -D-glucopyranosyl]-(1 \rightarrow 4)-N-acetylnormuramoyl-L- α -aminobutanoyl-D-isoglutamine, lipophilic disaccharide analogs of MDP

AU Ledvina, Miroslav; Jezek, Jan; Saman, David; Vaisar, Tomas; Hribalova, Vera

CS Inst. Org. Chem. Biochem., Czech. Acad. Sci., Prague, 166 10, Czech.

SO Carbohydrate Research (1994), 251, 269-84

CODEN: CRBRAT; ISSN: 0008-6215

DT Journal

LA English

OS CASREACT 121:36053

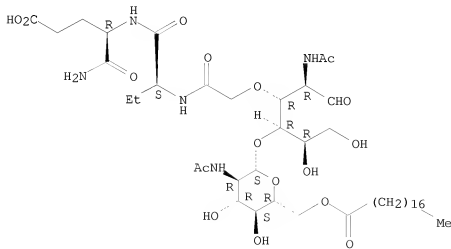
IT 155780-14-6P 155780-15-7P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation, pyrogenicity and adjuvant activity of)

RN 155780-14-6 HCAPLUS

CN Pentanoic acid, 4-[[[(2S)-2-[[[N-acetyl-4-O-[2-(acetyl-amino)-2-deoxy-6-O-(1-oxooctadecyl)- β -D-glucopyranosyl]normuramoyl]amino]-1-oxobutyl]amino]-5-amino-5-oxo-, (4R)- (9CI) (CA INDEX NAME)

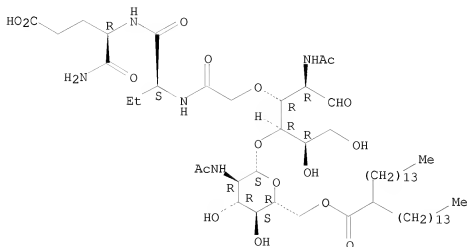
Absolute stereochemistry.



RN 155780-15-7 HCAPLUS

CN Pentanoic acid, 4-[[[2S]-2-[[N-acetyl-4-O-[2-(acetilamino)-2-deoxy-6-O-(1-oxo-2-tetradecylhexadecyl)-β-D-glucopyranosyl]normuramoyl]amino]-1-oxobutyl]amino]-5-amino-5-oxo-, (4R)- (9CI) (CA INDEX NAME)

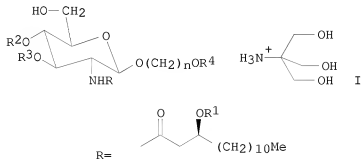
Absolute stereochemistry.



L33 ANSWER 9 OF 42 HCAPLUS COPYRIGHT 2008 ACS on STN

TI New acyclic analogs of lipid A: synthesis of 4-phosphonoxybutyl and 3-phosphonoxypropyl glycosides of 2-amino-2-deoxy-D-glucose

GI



AB Several analogs, I [n = 3, 4; R₂ = H, PO₃H-, R (R₁ = H); R₃ = R [R₁ = H, CO(CH₂)₁₂Me]; R₄ = H, PO₃H-] of lipid A have been synthesized, in which the reducing monosaccharide moiety of the parent mol. has been replaced by an acyclic spacer. The new compds. show high endotoxic activity and are able to protect neutropenic mice against pseudomonas infection, two properties characteristic of LPS-like mols.

AN 1994:436052 HCAPLUS <<LOGINID::20081210>>

DN 121:36052

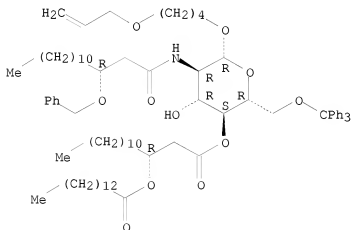
OREF 121:6683a,6686a

TI New acyclic analogs of lipid A: synthesis of 4-phosphonoxybutyl and 3-phosphonoxypropyl glycosides of 2-amino-2-deoxy-D-glucose

AU Eustache, Jacques; Grob, Alfred; Retscher, Hannelore

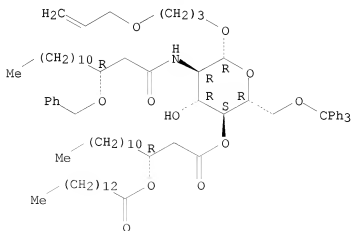
CS Sandoz Forschungsinst. Wien, Vienna, A-1235, Austria
 SO Carbohydrate Research (1994), 251, 251-67
 CODEN: CRBRAT; ISSN: 0008-6215
 DT Journal
 LA English
 IT 155739-65-4P 155739-66-5P
 RL: FORM (Formation, nonpreparative); PREP (Preparation)
 (formation of, in synthesis of lipid A analogs)
 RN 155739-65-4 HCAPLUS
 CN β -D-Glucopyranoside, 4-(2-propenyloxy)butyl
 2-deoxy-2-[[1-oxo-3-(phenylmethoxy)tetradecyl]amino]-6-O-(triphenylmethyl)-
 , 4-[3-[[1-oxotetradecyl]oxy]tetradecanoate], [2(R),4(R)]- (9CI) (CA
 INDEX NAME)

Absolute stereochemistry.



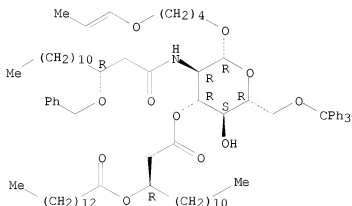
RN 155739-66-5 HCAPLUS
 CN β -D-Glucopyranoside, 3-(2-propenyloxy)propyl
 2-deoxy-2-[[1-oxo-3-(phenylmethoxy)tetradecyl]amino]-6-O-(triphenylmethyl)-
 , 4-[3-[[1-oxotetradecyl]oxy]tetradecanoate], [2(R),4(R)]- (9CI) (CA
 INDEX NAME)

Absolute stereochemistry.



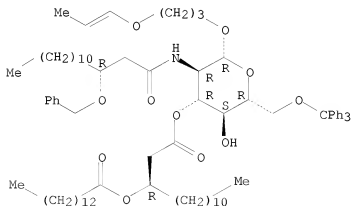
IT 155739-68-7P 155739-69-8P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation and hydrolysis of, in synthesis of lipid A analogs)
 RN 155739-68-7 HCAPLUS
 CN β -D-Glucopyranoside, 4-(1-propenyloxy)butyl
 2-deoxy-2-[[1-oxo-3-(phenylmethoxy)tetradecyl]amino]-6-O-(triphenylmethyl)-
 , 3-[3-[[1-oxotetradecyl]oxy]tetradecanoate], [2(R),3(R)]- (9CI) (CA
 INDEX NAME)

Absolute stereochemistry.
 Double bond geometry unknown.



RN 155739-69-8 HCAPLUS
 CN β -D-Glucopyranoside, 3-(1-propenyloxy)propyl
 2-deoxy-2-[[1-oxo-3-(phenylmethoxy)tetradecyl]amino]-6-O-(triphenylmethyl)-
 , 3-[3-[[1-oxotetradecyl]oxy]tetradecanoate], [2(R),3(R)]- (9CI) (CA
 INDEX NAME)

Absolute stereochemistry.
 Double bond geometry unknown.



IT 155739-45-0P 155739-47-2P 155739-48-3P
 155739-49-4P 155739-50-7P 155739-51-8P
 155739-52-9P 155751-71-6P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

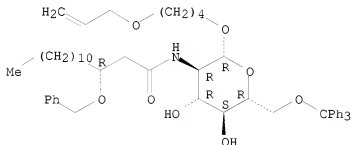
(Reactant or reagent)

(preparation and reaction of, in synthesis of lipid A analogs)

RN 155739-45-0 HCAPLUS

CN β -D-Glucopyranoside, 4-(2-propenyloxy)butyl
2-deoxy-2-[[1-oxo-3-(phenylmethoxy)tetradecyl]amino]-6-O-(triphenylmethyl)-
, (R)- (9CI) (CA INDEX NAME)

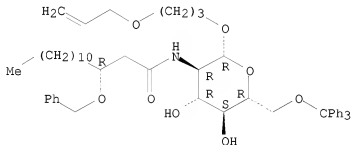
Absolute stereochemistry.



RN 155739-47-2 HCAPLUS

CN β -D-Glucopyranoside, 3-(2-propenyloxy)propyl
2-deoxy-2-[[1-oxo-3-(phenylmethoxy)tetradecyl]amino]-6-O-(triphenylmethyl)-
(9CI) (CA INDEX NAME)

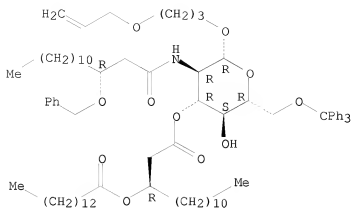
Absolute stereochemistry.



RN 155739-48-3 HCAPLUS

CN β -D-Glucopyranoside, 3-(2-propenyloxy)propyl
2-deoxy-2-[[1-oxo-3-(phenylmethoxy)tetradecyl]amino]-6-O-(triphenylmethyl)-
, 3-[3-[[1-oxotetradecyl]oxy]tetradecanoate], [2(R),3(R)]- (9CI) (CA
INDEX NAME)

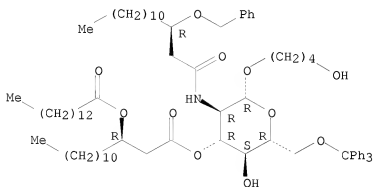
Absolute stereochemistry.



RN 155739-49-4 HCAPLUS

CN β -D-Glucopyranoside, 4-[[1-oxo-3-(phenylmethoxy)tetradecyl]amino]-6-O-(triphenylmethyl)-2-deoxy-2-[[1-oxo-3-(phenylmethoxy)tetradecyl]oxy]tetradecanoate, [2(R),3(R)]- (9CI) (CA INDEX NAME)

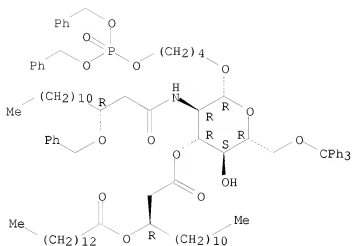
Absolute stereochemistry.



RN 155739-50-7 HCAPLUS

CN β -D-Glucopyranoside, 4-[[bis(phenylmethoxy)phosphinyl]oxy]butyl 2-deoxy-2-[[1-oxo-3-(phenylmethoxy)tetradecyl]amino]-6-O-(triphenylmethyl)-, 3-[[3-[[1-oxotetradecyl]oxy]tetradecanoate], [2(R),3(R)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

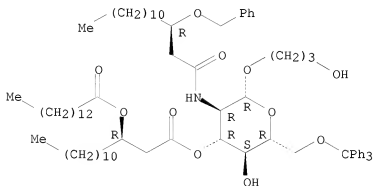


RN 155739-51-8 HCAPLUS

CN β -D-Glucopyranoside, 3-hydroxypropyl

2-deoxy-2-[[1-oxo-3-(phenylmethoxy)tetradecyl]amino]-6-O-(triphenylmethyl)-
 , 3-[3-[[1-oxotetradecyl]oxy]tetradecanoate], [2(R),3(R)]- (9CI) (CA
 INDEX NAME)

Absolute stereochemistry.

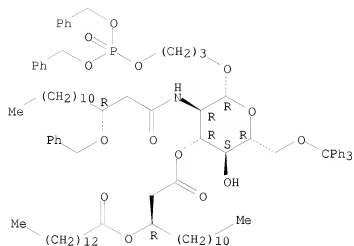


RN 155739-52-9 HCAPLUS

CN β -D-Glucopyranoside, 3-[[bis(phenylmethoxy)phosphinyl]oxy]propyl

2-deoxy-2-[[1-oxo-3-(phenylmethoxy)tetradecyl]amino]-6-O-(triphenylmethyl)-
 , 3-[3-[[1-oxotetradecyl]oxy]tetradecanoate], [2(R),3(R)]- (9CI) (CA
 INDEX NAME)

Absolute stereochemistry.

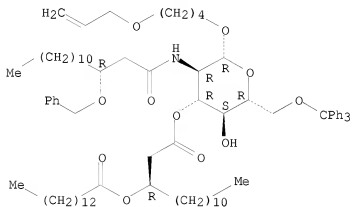


RN 155751-71-6 HCAPLUS

CN β -D-Glucopyranoside, 4-(2-propenyloxy)butyl

2-deoxy-2-[[1-oxo-3-(phenylmethoxy)tetradecyl]amino]-6-O-(triphenylmethyl)-
 , 3-[3-[(1-oxotetradecyl)oxy]tetradecanoate], [2(R),3(R)]- (9CI) (CA
 INDEX NAME)

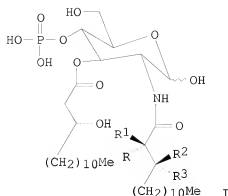
Absolute stereochemistry.



L33 ANSWER 10 OF 42 HCAPLUS COPYRIGHT 2008 ACS on STN

TI Syntheses of 2-deoxy-2-[(2R,3S)-2-fluoro-3-hydroxytetradecanamido]-3-O-
 [(3R)-3-hydroxytetradecanoyl]-4-O-phosphono-D-glucopyranose and its
 (2S,3R)-isomer

GI



AB Title compds. I (R = R₃ = H, R₂ = OH, R₃ = F; R = F, R₁ = R₂ = H, R₃ = OH) were prepared from allyl 2-[(2R,3S)-3-(benzyloxycarbonyloxy)-2-fluorotetradecanamido]-2-deoxy-4,6-O-isopropylidene-β-D-glucopyranoside and its corresponding (2S,3R) isomer. Compds. I did not activate macrophage, but the (2S,3R)-analog strongly inhibited the binding of LPS to macrophage.

AN 1994:192121 HCAPLUS <<LOGINID:20081210>>

DN 120:192121

OREF 120:34023a,34026a

TI Syntheses of 2-deoxy-2-[(2R,3S)-2-fluoro-3-hydroxytetradecanamido]-3-O-[(3R)-3-hydroxytetradecanoyl]-4-O-phosphono-D-glucopyranose and its (2S,3R)-isomer

AU Shiozaki, Masao; Arai, Masami; Hiraoka, Tetsuo; Nishijima, Masahiro; Akamatsu, Yuzuru

CS New Lead Res. Lab., Sankyo Co., Ltd., Tokyo, 140, Japan

SO Bioscience, Biotechnology, and Biochemistry (1993), 57(9), 1526-9

CODEN: BBBIEJ; ISSN: 0916-8451

DT Journal

LA English

IT 132760-39-5P

RL: SPN (Synthetic preparation); PREP (Preparation)

(intermediate in preparation of fluorohydroxyamidoglucopyranoses)

RN 132760-39-5 HCAPLUS

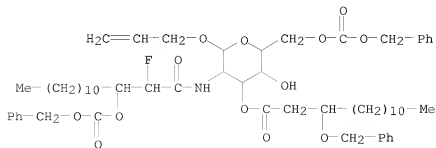
CN β-D-Glucopyranoside, 2-propenyl

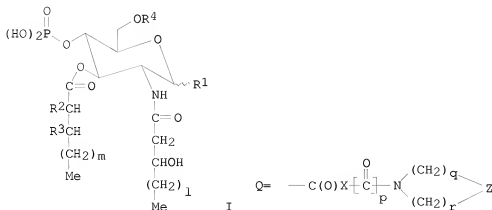
2-deoxy-2-[[2-fluoro-1-oxo-3-

[(phenylmethoxy)carbonyl]oxy]tetradecyl]amino]-,

3-[3-(phenylmethoxy)tetradecanoate] 6-(phenylmethyl carbonate),

[2(2S,3R),3(R)]- (9CI) (CA INDEX NAME)





AB The title compds. [I; $R^1 = H$, HO ; one of R^2 and $R^3 = O_2C(CH_2)_nMe$, $CH_2(CH_2)_nMe$, or $OCH_2(CH_2)_nMe$, and the other = H ; $R^4 = C(O)X(CO)pY$, $Q = (un)substituted$ linear or branched lower alkylene; $Y = (un)substituted$ NH_2 ; $Z = (un)substituted$ NH or CH_2 , O ; $l, m, n = 4-16$; $p = 0,1$; $q = 0-4$; $r = 1-3$], having lipid A-like activities and useful as antitumor agents and immunostimulants, are prepared. Thus, amidation of 2-amino-1,5-anhydro-2-deoxy-4,6-O-isopropylidene-D-glucitol with (R)-3-[2-(trimethylsilyl)ethoxymethoxy]tetradecanoic acid in the presence of 1-ethyl-2,3-(diethylaminopropyl)carbodiimide (WSC)-HCl in CH_2Cl_2 followed by esterification with (R)-2-dodecylhexadecanoic acid in the presence of 4-dimethylaminopyridine (DMAP) and WSC.HCl in CH_2Cl_2 and deisopropylidenation with 95% aqueous AcOH at 50° gave 1,5-anhydro-2-deoxy-3-O-[(2RS)-2-dodecylhexadecanoyl]-2-[(3R)-3-[2-(trimethylsilyl)ethoxymethoxy]tetradecanamido]-D-glucitol (II). Esterification of II with $Me_2NCH_2CO_2H$ in the presence of WSC.HCl and DMAP in CH_2Cl_2 followed by sulfonylation with $(PhO)_2P(O)Cl$ in the presence of DMAP and WSC.HCl in CH_2Cl_2 gave, after deprotection with $Et_2O.BF_3$ and hydrolysis over PtO_2 in AcOH, I [$R^1 = R^3 = H$, $R^2 = (CH_2)_{11}Me$, $R^4 = COCH_2NMe_2$, $l = 10$, $m = 12$]. I [$R^1 = R^3 = H$, $R^2 = (CH_2)_{11}Me$, $R^4 = (S)-COCHMeNH_2$, $l = m = 10$] at $10 \mu g/mouse$ i.v. increased the production of TNF from <10 (control) to $421,283$ U/mL in mice treated i.v. with a first stimulant, *Corynebacterium parvum*. A total of 19 I were prepared

AN 1993:560726 HCAPLUS <<LOGINID:20081210>>

DN 119:160726

OREF 119:28829a, 28832a

TI Preparation of 6-aminoacyl-substituted lipid A analogs

IN Hasegawa, Akira; Kiso, Makoto; Agari, Shinichi; Ishida, Tomio; Goto, Hiroyuki; Waga, Iwao

PA Nippon Tobacco Sangyo, Japan

SO Jpn. Kokai Tokkyo Koho, 38 pp.

CODEN: JKXXAF

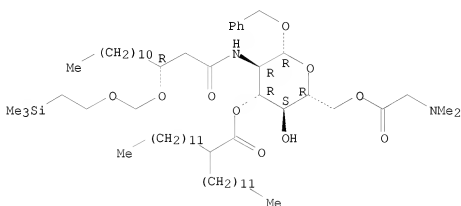
DT Patent

LA Japanese

FAN.CNT 1

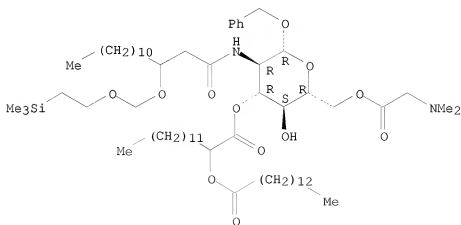
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 05059079	A	19930309	JP 1991-296695	19910827 <--
PRAI	JP 1991-296695		19910827	<--	
OS	MARPAT 119:160726				
IT	149895-83-0P 149924-02-7P				
	RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of, as intermediate for lipid A analog)				
RN	149895-83-0 HCAPLUS				
CN	Glycine, N,N-dimethyl-, 6-ester with phenylmethyl 2-deoxy-2-[[1-oxo-3-[[2-(trimethylsilyl)ethoxy]methoxy]tetradecyl]amino]- β-D-glucopyranoside 3-(2-dodecyltetradecanoate), (R)- (9CI) (CA INDEX NAME)				

Absolute stereochemistry.



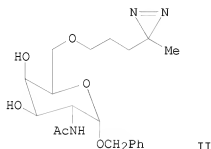
RN	149924-02-7 HCAPLUS
CN	Glycine, N,N-dimethyl-, 6-ester with phenylmethyl 2-deoxy-2-[[1-oxo-3-[[2-(trimethylsilyl)ethoxy]methoxy]tetradecyl]amino]- β-D-glucopyranoside 3-[2-[(1-oxotetradecyl)oxy]tetradecanoate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L33 ANSWER 12 OF 42 HCAPLUS COPYRIGHT 2008 ACS on STN
 TI Building units of oligosaccharides. CII. Synthesis of modified derivatives of 2-acetamido-2-deoxy-D-galactose for examination of substrate specificities of core 1- β 3-Gal-transferase and core 3- β 3-GlcNAc-transferase involved in the biosynthesis of O-glycoproteins

GI



AB The 2-, 3-, 4-, and 6-deoxy derivative of benzyl 2-acetamido-2-deoxy- α -D-galactopyranoside have been synthesized to test substrate specificities of the title glycosyltransferases. The core 1 β 3-gal-transferase (I) does not require the 6-OH group for activity in contrast to the core 3- β 3-GlcNAc-transferase which requires the 6-OH group. Compds. with reactive groups replacing the 6-OH group, such as the diazirine II, may be suitable for photolabeling I. A column for affinity chromatog. with the 6-deoxy derivative as the ligand may be useful for separating the two enzymes during purification

AN 1993:169478 HCAPLUS <<LOGINID:20081210>>

Correction of: 1992:408334

DN 118:169478

Correction of: 117:8334

OREF 118:29081a,29084a

TI Building units of oligosaccharides. CII. Synthesis of modified derivatives of 2-acetamido-2-deoxy-D-galactose for examination of substrate specificities of core 1- β 3-Gal-transferase and core 3- β 3-GlcNAc-transferase involved in the biosynthesis of O-glycoproteins

AU Paulsen, Hans; Rutz, Volker; Brockhausen, Inka

CS Inst. Org. Chem., Univ. Hamburg, Hamburg, W-2000/13, Germany

SO Liebigs Annalen der Chemie (1992), (7), 735-45

CODEN: LACHDL; ISSN: 0170-2041

DT Journal

LA German

OS CASREACT 118:169478

IT 141019-96-7P

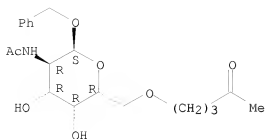
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and reaction of, with hydroxylaminesulfonic acid)

RN 141019-96-7 HCAPLUS

CN α -D-Galactopyranoside, phenylmethyl

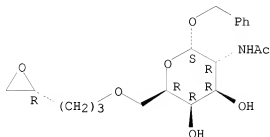
2-(acetylamino)-2-deoxy-6-O-(4-oxopentyl)- (CA INDEX NAME)

Absolute stereochemistry.



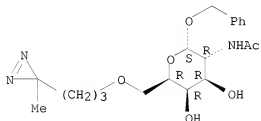
IT 141019-94-5P 141019-97-8P 141020-05-5P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of, as glycosyl transferase substrate)
 RN 141019-94-5 HCAPLUS
 CN α -D-Galactopyranoside, phenylmethyl
 2-(acetylamino)-2-deoxy-6-O-(3-oxiranylpropyl)-, (R)- (9CI) (CA INDEX
 NAME)

Absolute stereochemistry.



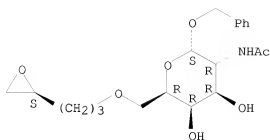
RN 141019-97-8 HCAPLUS
 CN α -D-Galactopyranoside, phenylmethyl
 2-(acetylamino)-2-deoxy-6-O-[3-(3-methyl-3H-diazirin-3-yl)propyl]- (CA
 INDEX NAME)

Absolute stereochemistry.

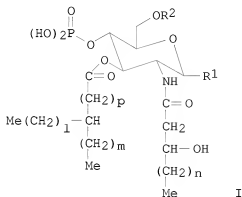


RN 141020-05-5 HCAPLUS
 CN α -D-Galactopyranoside, phenylmethyl
 2-(acetylamino)-2-deoxy-6-O-(3-oxiranylpropyl)-, (S)- (9CI) (CA INDEX
 NAME)

Absolute stereochemistry.



L33 ANSWER 13 OF 42 HCAPLUS COPYRIGHT 2008 ACS on STN
 TI Preparation of 6-substituted lipid A analogs as immunostimulants and
 antitumor agents
 GI



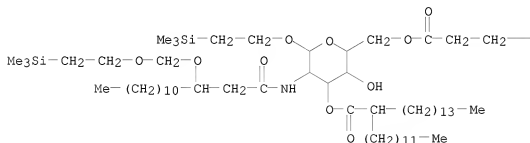
AB The title compds. [I; R1 = H, OH; R2 = COR3; R3 = CO2H or lower
 alkoxy carbonyl-substituted) linear or branched lower alkyl; l = 5-17; m =
 7-19; n = 4-16; p = 0,1] are prepared Thus, acylation of
 2-amino-1,5-anhydro-2-deoxy-4,6-O-isopropylidene-D-glucitol with
 (R)-3-[2-(trimethylsilyl)ethoxymethoxy]tetradecanoic acid followed by
 (R,S)-2-dodecylhexadecanoic acid in the presence of
 1-ethyl-3-(3-dimethylaminopropyl)carbodiimide hydrochloride in CH2Cl2 gave
 N,O -diacyl derivative which was treated with 95% AcOH at 50 °,
 6-acylated with 3-(methoxycarbonyl)propionyl chloride in the presence of
 pyridine in CHCl3, 4-phosphorylated with (PhO)2POCl in the presence of
 pyridine in CH2Cl2, and then deprotected with BF3.Et2O to give I [R1 = H,
 R2 = CO(CH2)2CO2Me, l = 11, m = 13, n = 10, p = 0]. This in vivo enhanced
 the production of tumor necrosis factor from <10 U/mL (control) in serum to
 727,800 U/mL in mice treated with Corynebacterium parvum i.v.

AN 1993:147982 HCAPLUS <<LOGINID::20081210>>
 DN 118:147982
 OREF 118:25459a,25462a
 TI Preparation of 6-substituted lipid A analogs as immunostimulants and
 antitumor agents
 IN Hasegawa, Akira; Kiso, Makoto; Agari, Shinichi; Ishida, Tomio; Suzuki,

PA Masanobu; Saito, Yutaka
 SO Japan Tobacco, Inc., Japan
 SO Jpn. Kokai Tokkyo Koho, 30 pp.
 CODEN: JKXXAF
 DT Patent
 LA Japanese
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 04234895	A	19920824	JP 1991-115723	19910227 <--
	WO 9311139	A1	19930610	WO 1991-JP1628	19911127 <--
	W: CA, KR, US				
	RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LU, NL, SE				
EP	593765	A1	19940427	EP 1991-920691	19911127 <--
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
PRAI	JP 1990-45483	A1	19900228	<--	
	WO 1991-JP1628	W	19911127	<--	
OS	MARPAT 118:147982				
IT	146371-05-3P 146371-17-7P				
	RL: SPN (Synthetic preparation); PREP (Preparation)				
	(preparation of, as intermediate for lipid A analog immunostimulant and antitumor agent)				
RN	146371-05-3 HCAPLUS				
CN	β -D-Glucopyranoside, 2-(trimethylsilyl)ethyl 2-deoxy-2-[[1-oxo-3-[[2-(trimethylsilyl)ethoxy]methoxy]tetradecyl]amino]-, 3-(2-dodecylhexadecanoate) 6-(methyl butanedioate) (9CI) (CA INDEX NAME)				

PAGE 1-A

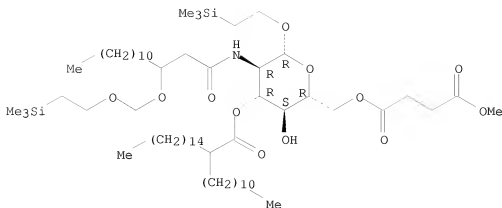


PAGE 1-B

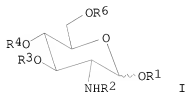


RN 146371-17-7 HCAPLUS
 CN β -D-Glucopyranoside, 2-(trimethylsilyl)ethyl
 2-deoxy-2-[[1-oxo-3-[[2-(trimethylsilyl)ethoxy]methoxy]tetradecyl]amino]-,
 6-(methyl butanedioate) 3-(2-undecylheptadecanoate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L33 ANSWER 14 OF 42 HCAPLUS COPYRIGHT 2008 ACS on STN
 TI Preparation of lipid X analogs as immunostimulants and antitumor agents
 GI



AB The title compds. [I; one of R1, R4 = H, P(O)(OH)2, OH-protecting group, and the other = P(O)(OH)2; R2, R3 = (un)substituted C6-20 acyl; R6 = H, OH-protecting group; provided that both R2 and R3 ≠ (HO- or C2-20 acyl-substituted) C6-20 acyl], having excellent macrophage-activating activity with little toxicity, are prepared Thus, acylation of allyl 2-deoxy-2-amino-4,6-isopropylidene-β-D-glucopyranoside with (R)-3-benzoyloxymyristic acid followed by (±)-syn-2-fluoro-3-benzoyloxycarbonyloxymyristic acid in the presence of DCC in CH2Cl2 gave β-I [R1 = allyl, R2 = (3'R)-3'-benzoyloxymyristoylamino, R3 = (2''RS,3''SR)-2''-fluoro-3''-(benzoyloxycarbonyloxy)myristoyl, R4R6 = isopropylidene] which was deprotected with 1,5-cyclooctadiene-bis(methyldiphenylphosphine)iridium hexafluorophosphate, H2O, iodine, and pyridine in THF to give I [R1 = OH, (2''RS,3''SR)-2''-fluoro-3''-(benzoyloxycarbonyloxy)myristoyl, R4R6 = isopropylidene]. This was acylated with (PhCH2O)2POCl in the presence of BuLi in THF at -78° followed by hydrogenolysis over 10% Pd-C at -78° and simultaneous deacetonation to give I [R1 = P(O)(OH)2, R2 = (3'R)-3'-benzoyloxymyristoylamino, R3 = (2''RS,3''SR)-2''-fluoro-3''-(benzoyloxycarbonyloxy)myristoyl, R4 = R6 = H]. When I [R1 = R6 = H, R2 = COCH2(OH)C11H23, R3 = COCHF(O2CC13H27)C11H23, R4 = P(O)(OH)2] (sic) was incubated for 18 h with [14C]-arachidonic acid in animal cells [J. Bio. Chemical, volume 262(35) page 17, 212-17, 220], the count of labeled prostaglandin, which was correlated to macrophage activity, was 185/min.

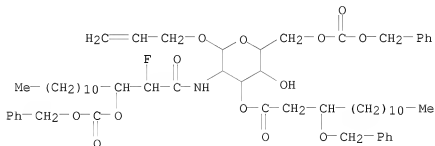
AN 1993:147981 HCAPLUS <<LOGINID:20081210>>
 DN 118:147981
 OREF 118:25459a,25462a
 TI Preparation of lipid X analogs as immunostimulants and antitumor agents
 IN Shiosaki, Masao; Ishida, Noboru; Arai, Masami; Kobayashi, Tomoo; Hiraoka,
 Tetsuo; Nishijima, Masahiro; Akamatsu, Minoru
 PA Sankyo Co., Ltd., Japan
 SO Jpn. Kokai Tokkyo Koho, 38 pp.
 CODEN: JKXXAF
 DT Patent
 LA Japanese
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 04235193	A	19920824	JP 1991-147075	19910619 <--
	JP 3040847	B2	20000515		
PRAI	JP 1990-164646	A1	19900622	<--	
OS	MARPAT 118:147981				
IT	132760-39-5P 132828-16-1P 132882-54-3P 138527-79-4P				

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of, as intermediate for immunostimulant and antitumor lipid X
 analog)

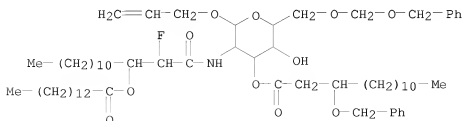
RN 132760-39-5 HCAPLUS

CN β -D-Glucopyranoside, 2-propenyl
 2-deoxy-2-[[2-fluoro-1-oxo-3-
 [[(phenylmethoxy)carbonyl]oxy]tetradecyl]amino]-,
 3-[3-(phenylmethoxy)tetradecanoate] 6-(phenylmethyl carbonate),
 [2(2S,3R),3(R)]- (9CI) (CA INDEX NAME)



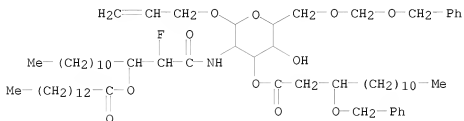
RN 132828-16-1 HCAPLUS

CN β -D-Glucopyranoside, 2-propenyl
 2-deoxy-2-[[2-fluoro-1-oxo-3-[[1-oxotetradecyl]oxy]tetradecyl]amino]-6-O-
 [(phenylmethoxy)methyl]-, 3-[3-(phenylmethoxy)tetradecanoate],
 [2(2S,3R),3(R)]- (9CI) (CA INDEX NAME)



RN 132882-54-3 HCAPLUS

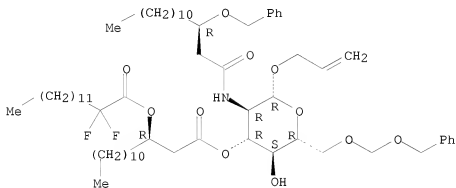
CN β -D-Glucopyranoside, 2-propenyl
2-deoxy-2-[[2-fluoro-1-oxo-3-[(1-oxotetradecyl)oxy]tetradecyl]amino]-6-O-
[(phenylmethoxy)methyl]-, 3-[3-(phenylmethoxy)tetradecanoate],
[2(2R,3S),3(R)]- (9CI) (CA INDEX NAME)



RN 138527-79-4 HCAPLUS

CN β -D-Glucopyranoside, 2-propenyl
2-deoxy-2-[[1-oxo-3-(phenylmethoxy)tetradecyl]amino]-6-O-
[(phenylmethoxy)methyl]-, 3-[3-[(2,2-difluoro-1-oxotetradecyl)oxy]tetradecanoate], [2(R),3(R)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L33 ANSWER 15 OF 42 HCAPLUS COPYRIGHT 2008 ACS on STN

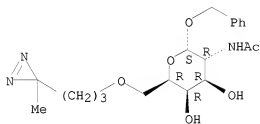
TI Control of O-glycan synthesis: specificity and inhibition of O-glycan
core 1 UDP-galactose:N-acetylgalactosamine- α -R
 β 3-galactosyltransferase from rat liver

AB The specificity of glycosyltransferases is a major control factor in the
biosynthesis of O-glycans. The enzyme that synthesizes O-glycan core 1,
i.e., UDP-galactose:N-acetylgalactosamine- α -R
 β 3-galactosyltransferase (β 3-Gal-T; EC 2.4.1.122), was partially
purified from rat liver. The enzyme preparation, free of pyrophosphatases,
 β 4-galactosyl-transferase, β -galactosidase, and
N-acetylglucosaminyltransferase I, was used to study the specificity and
inhibition of the β 3-Gal-T. β 3-Gal-T activity is sensitive to
changes in the R-group of the GalNAc-R acceptor substrate and is
stimulated when the R-group is a peptide or an aromatic group. Derivs. of
GalNAc-benzyl were synthesized and tested as potential substrates
and inhibitors. Removal or substitution of the 3-hydroxyl or removal of
the 4-hydroxyl of GalNAc abolished β 3-Gal-T activity. Comps. with

modifications of the 3- or 4-hydroxyl of GalNAc α -benzyl did not show significant inhibition. Removal or substitution of the 6-hydroxyl of GalNAc reduced activity slightly and these derivs. acted as competitive substrates. Derivs. with epoxide groups attached to the 6-position of GalNAc acted as substrates and not as inhibitors, with the exception of the photosensitive 6-O-(4,4-azo)phenyl-GalNAc α -benzyl, which inhibited Gal incorporation into GalNAc-benzyl. The results indicate that the enzyme does not require the 6-hydroxyl of GalNAc, but needs the 3- and the axial 4-hydroxyl as essential requirements for binding and activity. In the usual biochem. O-glycan pathway, core 2 (GlcNAc β 6[Gal β 3]GalNAc α -R) is formed from core 1 (Gal β 3GalNAc-R). Thus an alternate pathway has been demonstrated that may be of importance in human tissues.

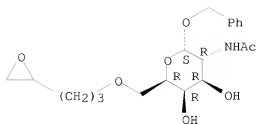
AN 1992:507008 HCAPLUS <<LOGINID:20081210>>
 DN 117:107008
 OREF 117:18545a,18548a
 TI Control of O-glycan synthesis: specificity and inhibition of O-glycan core 1 UDP-galactose:N-acetylgalactosamine- α -R β 3-galactosyltransferase from rat liver
 AU Brockhausen, Inka; Moller, Gabriele; Pollex-Kruger, Annette; Rutz, Volker; Paulsen, Hans; Matta, Khushi L.
 CS Res. Inst., Hosp. Sick Child., Toronto, ON, M5G 1X8, Can.
 SO Biochemistry and Cell Biology (1992), 70(2), 99-108
 CODEN: BCBIEQ; ISSN: 0829-8211
 DT Journal
 LA English
 IT 141019-97-8 142925-54-0
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with UDP-galactose-acetylgalactosamine
 galactosyltransferase of liver, substrate structure in relation to)
 RN 141019-97-8 HCAPLUS
 CN α -D-Galactopyranoside, phenylmethyl
 2-(acetylamino)-2-deoxy-6-O-[3-(3-methyl-3H-diazirin-3-yl)propyl]- (CA INDEX NAME)

Absolute stereochemistry.



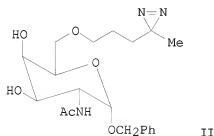
RN 142925-54-0 HCAPLUS
 CN α -D-Galactopyranoside, phenylmethyl
 2-(acetylamino)-2-deoxy-6-O-(3-oxiranylpropyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L33 ANSWER 16 OF 42 HCAPLUS COPYRIGHT 2008 ACS on STN
 TI Building units of oligosaccharides. CII. Synthesis of modified derivatives of 2-acetamido-2-deoxy-D-galactose for examination of substrate specificities of core 1- β -Gal-transferase and core 3- β -GlcNAc-transferase involved in the biosynthesis of O-glycoproteins

GI



AB The 2-, 3-, 4-, and 6-deoxy derivs. of benzyl 2-acetamido-2-deoxy- α -D-galactopyranoside have been synthesized to test substrate specificities of the title glycosyltransferases. The core 1 β -gal-transferase (I) does not require the 6-OH group for activity in contrast to the core 3- β -GlcNAc-transferase which requires the 6-OH group. Compds. with reactive groups replacing the 6-OH group such as the diazirine II could be suitable for photolabeling of the former enzyme. A column for affinity chromatog. with the 6-deoxy derivative as the ligand could be useful for separating the two enzymes during purification

AN 1992:408334 HCAPLUS <<LOGINID::20081210>>

DN 117:8334

OREF 117:1687a,1690a

TI Building units of oligosaccharides. CII. Synthesis of modified derivatives of 2-acetamido-2-deoxy-D-galactose for examination of substrate specificities of core 1- β -Gal-transferase and core 3- β -GlcNAc-transferase involved in the biosynthesis of O-glycoproteins

AU Paulsen, Hans; Rutz, Volker; Brockhausen, Inka

CS Inst. Org. Chem., Univ. Hamburg, Hamburg, W-2000/13, Germany

SO Liebigs Annalen der Chemie (1992), (5), 513-21

CODEN: LACHDL; ISSN: 0170-2041

DT Journal

LA German

IT 141019-96-7P

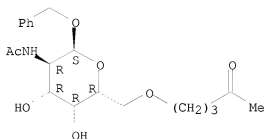
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reaction of, with hydroxylaminesulfonic acid)

RN 141019-96-7 HCAPLUS

CN α -D-Galactopyranoside, phenylmethyl
2-(acetylamino)-2-deoxy-6-O-(4-oxopentyl)- (CA INDEX NAME)

Absolute stereochemistry.



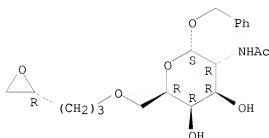
IT 141019-94-5P 141019-97-8P 141020-05-5P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as glycosyltransferase substrate)

RN 141019-94-5 HCAPLUS

CN α -D-Galactopyranoside, phenylmethyl
2-(acetylamino)-2-deoxy-6-O-(3-oxiranylpropyl)-, (R)- (9CI) (CA INDEX NAME)

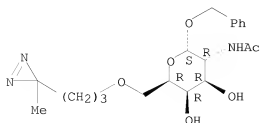
Absolute stereochemistry.



RN 141019-97-8 HCAPLUS

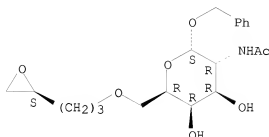
CN α -D-Galactopyranoside, phenylmethyl
2-(acetylamino)-2-deoxy-6-O-[3-(3-methyl-3H-diazirin-3-yl)propyl]- (CA INDEX NAME)

Absolute stereochemistry.

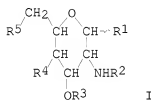


RN 141020-05-5 HCAPLUS
 CN α -D-Galactopyranoside, phenylmethyl
 2-(acetamino)-2-deoxy-6-O-(3-oxiranylpropyl)-, (S)- (9CI) (CA INDEX
 NAME)

Absolute stereochemistry.



L33 ANSWER 17 OF 42 HCAPLUS COPYRIGHT 2008 ACS on STN
 TI Preparation of lipid A analogs as immunostimulants and antitumor activity
 GI



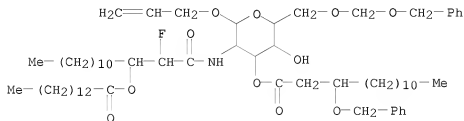
AB The title compds. [I; R1, R5 = (protected) OH, F, OP(O)(OH)₂; R2, R3 = (substituted) aliphatic acyl; R4 = (protected) OH, OP(O)(OH)₂; with provisos] were prepared. Allyl 2-deoxy-2-amino-4,6-O-isopropylidene- β -D-glucopyranoside (preparation given) was condensed with (R)-3-benzoyloxytetradecanoic acid in CH₂Cl₂ containing DCC to give allyl 2-deoxy-2-[(3R)-3'-benzyloxytetradecanoylamino]-4,6-O-isopropylidene- β -D-glucopyranoside, which was further condensed with (+)-syn-2-fluoro-3-benzoyloxycarbonyloxytetradecanoic acid to give allyl 2-deoxy-2-[(3R')-3'-benzyloxytetradecanoylamino]-3-O-[(2''RS,3''SR)-2''-fluoro-3''-(benzyloxycarbonyloxy)tetradecanoyl]-4,6-O-isopropylidene- β -D-glucopyranoside, which in THF was treated with 1,5-cyclohexadienebis[methyldiphenylphosphine]iridium hexafluorophosphate to give 2-deoxy-2-[(3R)-3'-benzyloxytetradecanoylamino]-3-O-[(2''RS,3''SR)-2''-fluoro-3''-(benzyloxycarbonyloxy)tetradecanoyl]-4,6-O-isopropylidene-D-glucopyranose. This was phosphorylated with dibenzyl phosphorochloridate in THF-hexane containing BuLi to give, after hydrogenolysis over Pd/C, 2-deoxy-2-[(3R)-3'-hydroxytetradecanoylamino]-3-O-[(2''RS,3''SR)-2''-fluoro-3''-hydroxytetradecanoyl]- α -D-glucopyranose 1-phosphate. In an in vitro experiment comparing the ability of I to effect release of [14C]-prostaglandin D₂ using a macrophage-like mouse cell line J774.1, 2-deoxy-2-[(2'S,3'R)-2'-fluoro-3'-hydroxytetradecanoylamino]-3-O-[(3'R)-tetradecanoyloxy]tetradecanoyl-4,6-O-isopropylidene- α -D-glucopyranose 4-phosphate (prepared similarly) was 18% more active than the

known GLA-60.
AN 1992:214840 HCAPLUS <<LOGINID:20081210>>
DN 116:214840
OREF 116:36429a,36432a
TI Preparation of lipid A analogs as immunostimulants and antitumor activity
IN Shiozaki, Masao; Ishida, Noboru; Kobayashi, Tomowo; Hiraoka, Tetsuo; Arai,
Masami; Akamatsu, Yuzuru; Nishijima, Masahiro
PA Sankyo Co., Ltd., Japan
SO Eur. Pat. Appl., 130 pp.
CODEN: EPXXDW
DT Patent
LA English
FAN.CNT 2

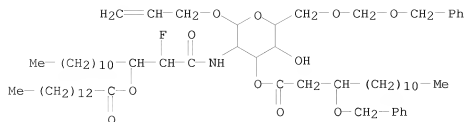
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 437016	A2	19910717	EP 1990-307045	19900627 <--
	EP 437016	B1	19960501		
	R: AT, BE, CH, DE, DK, ES, FR, GB, IT, LU, NL, SE				
	JP 02256697	A	19901017	JP 1989-321153	19891211 <--
	JP 2839921	B2	19981224		
	JP 03291292	A	19911220	JP 1990-401087	19901210 <--
	JP 2980693	B2	19991122		
PRAI	JP 1989-321153	A	19891211	<--	
	JP 1990-73739	A	19900220	<--	
	JP 1988-329964	A1	19881227	<--	

OS MARPAT 116:214840
IT 132828-16-1P 132882-54-3P 138527-59-0P
138527-79-4P 138527-88-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as intermediate for lipid A analogs)

RN 132828-16-1 HCAPLUS
CN β -D-Glucopyranoside, 2-propenyl
2-deoxy-2-[[2-fluoro-1-oxo-3-[(1-oxotetradecyl)oxy]tetradecyl]amino]-6-O-
[(phenylmethoxy)methyl]-, 3-[3-(phenylmethoxy)tetradecanoate],
[2(2S,3R),3(R)]- (9CI) (CA INDEX NAME)



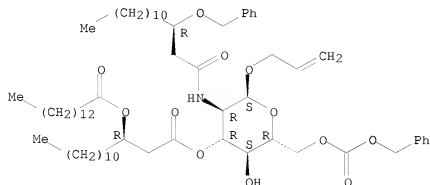
RN 132882-54-3 HCAPLUS
CN β -D-Glucopyranoside, 2-propenyl
2-deoxy-2-[[2-fluoro-1-oxo-3-[(1-oxotetradecyl)oxy]tetradecyl]amino]-6-O-
[(phenylmethoxy)methyl]-, 3-[3-(phenylmethoxy)tetradecanoate],
[2(2R,3S),3(R)]- (9CI) (CA INDEX NAME)



RN 138527-59-0 HCAPLUS

CN α -D-Glucopyranoside, 2-propenyl
2-deoxy-2-[[1-oxo-3-(phenylmethoxy)tetradecyl]amino]-,
3-[3-[(1-oxotetradecyl)oxy]tetradecanoate] 6-(phenylmethyl carbonate),
[2(R),3(R)]- (9CI) (CA INDEX NAME)

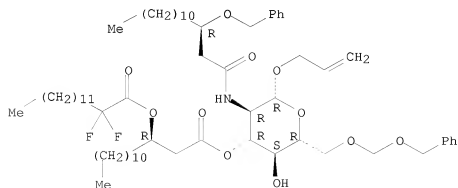
Absolute stereochemistry.



RN 138527-79-4 HCAPLUS

CN β -D-Glucopyranoside, 2-propenyl
2-deoxy-2-[[1-oxo-3-(phenylmethoxy)tetradecyl]amino]-6-O-
[(phenylmethoxy)methyl]-, 3-[3-[(2,2-difluoro-1-
oxotetradecyl)oxy]tetradecanoate], [2(R),3(R)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

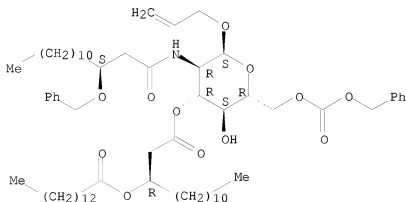


RN 138527-88-5 HCAPLUS

CN α -D-Glucopyranoside, 2-propenyl

2-deoxy-2-[[1-oxo-3-(phenylmethoxy)tetradecyl]amino]-,
 3-[3-[(1-oxotetradecyl)oxy]tetradecanoate] 6-(phenylmethyl carbonate),
 [2(S),3(R)]- (9CI) (CA INDEX NAME)

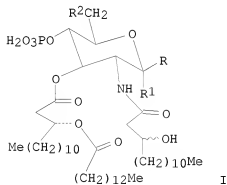
Absolute stereochemistry.



L33 ANSWER 18 OF 42 HCAPLUS COPYRIGHT 2008 ACS on STN

TI Syntheses of 2,6-dideoxy-6-fluoro-2-[(3R and 3S)-3-hydroxytetradecanamido]-3-O-[(3R)-3-(tetradecanoyloxy)-tetradecanoyl]-D-glucopyranose 4-(dihydrogen phosphate) and 2-deoxy-2-[(3R and 3S)-3-hydroxytetradecanamido]-3-O-[(3R)-3-(tetradecanoyloxy)tetradecanoyl]-α-D-glucopyranosyl fluoride 4-(dihydrogen phosphate): fluorosugar analogs of GLA-60

GI



AB Fluoro sugar analogs of GLA-60, e.g. I (RR1 = H, OH, R2 = F; R = H, R1 = F, R2 = OH), were synthesized from allyl 2-deoxy-4,6-O-isopropylidene-2-trifluoroacetamido-α-D-glucopyranoside.

AN 1992:174611 HCAPLUS <<LOGINID:20081210>>

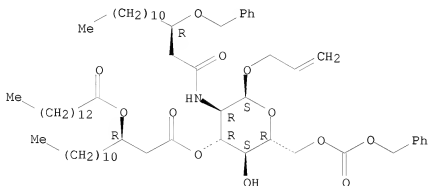
DN 116:174611

OREF 116:29575a,29578a

TI Syntheses of 2,6-dideoxy-6-fluoro-2-[(3R and 3S)-3-hydroxytetradecanamido]-3-O-[(3R)-3-(tetradecanoyloxy)-tetradecanoyl]-D-glucopyranose 4-(dihydrogen phosphate) and 2-deoxy-2-[(3R

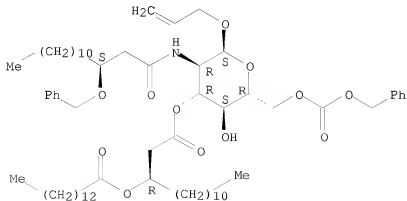
and 3S)-3-hydroxytetradecanamido]-3-O-[(3R)-3-(
 (tetradecanoyloxy)tetradecanoyl]- α -D-glucopyranosyl fluoride
 4-(dihydrogen phosphate): fluorosugar analogs of GLA-60
 AU Kobayashi, Yoshiyuki; Ishida, Nobory; Arai, Masami; Shiozaki, Masao;
 Hiraoka, Tetsuo; Nishijima, Masahiro; Kuge, Sayuri; Otsuka, Toshiaki;
 Akamatsu, Yuzuru
 CS New Lead Res. Lab., Sankyo Co. Ltd., Tokyo, 140, Japan
 SO Carbohydrate Research (1991), 222, 83-97
 CODEN: CRBRAT; ISSN: 0008-6215
 DT Journal
 LA English
 OS CASREACT 116:174611
 IT 138527-59-0P 138527-88-5P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation and phosphorylation of)
 RN 138527-59-0 HCAPLUS
 CN α -D-Glucopyranoside, 2-propenyl
 2-deoxy-2-[[1-oxo-3-(phenylmethoxy)tetradecyl]amino]-,
 3-[3-[(1-oxotetradecyl)oxy]tetradecanoate] 6-(phenylmethyl carbonate),
 [2(R),3(R)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

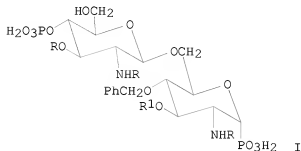


RN 138527-88-5 HCAPLUS
 CN α -D-Glucopyranoside, 2-propenyl
 2-deoxy-2-[[1-oxo-3-(phenylmethoxy)tetradecyl]amino]-,
 3-[3-[(1-oxotetradecyl)oxy]tetradecanoate] 6-(phenylmethyl carbonate),
 [2(S),3(R)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

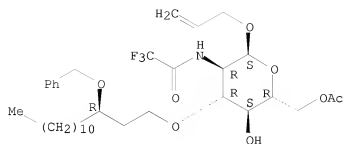


L33 ANSWER 19 OF 42 HCAPLUS COPYRIGHT 2008 ACS on STN
 TI Synthesis of a 3-ether analog of lipid A
 GI



AB Lipid A 3-ether analogs, e.g. I [R = (R)-3-(hydroxy)tetradecanoyl, R1 = (RS)-3-(hydroxy)decanoyl], were synthesized from allyl 2-deoxy-4,6-O-isopropylidene-2-trifluoroacetamido-α-D-glucopyranoside and 3,4,6-tri-O-acetyl-2-trifluoroacetamido-α-D-glucopyranosyl bromide. Compound I showed any endotoxic activity.
 AN 1992:152232 HCAPLUS <<LOGINID:20081210>>
 DN 116:152232
 OREF 116:25785a,25788a
 TI Synthesis of a 3-ether analog of lipid A
 AU Shiozaki, Masao; Kobayashi, Yoshiyuki; Arai, Masami; Ishida, Noboru; Hiraoka, Tetsuo; Nishijima, Masahiro; Kuge, Sayuri; Otsuka, Toshiaki; Akamatsu, Yuzuru
 CS New Lead Res. Lab., Sankyo Co., Ltd., Tokyo, 140, Japan
 SO Carbohydrate Research (1991), 222, 69-82
 CODEN: CRBRAT; ISSN: 0008-6215
 DT Journal
 LA English
 OS CASREACT 116:152232
 IT 137014-95-0P 139629-66-6P 139629-81-5P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and benzylation of)
 RN 137014-95-0 HCAPLUS
 CN α-D-Glucopyranoside, 2-propenyl 2-deoxy-3-O-[3-(phenylmethoxy)tetradecyl]-2-[(trifluoroacetyl)amino]-, 6-acetate, (R)- (9CI) (CA INDEX NAME)

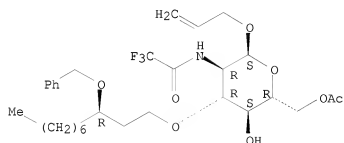
Absolute stereochemistry.



RN 139629-66-6 HCAPLUS

CN α -D-Glucopyranoside, 2-propenyl
2-deoxy-3-O-[3-(phenylmethoxy)decyl]-2-[(trifluoroacetyl)amino]-,
6-acetate, (R)- (9CI) (CA INDEX NAME)

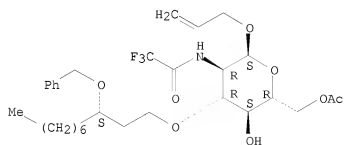
Absolute stereochemistry.



RN 139629-81-5 HCAPLUS

CN α -D-Glucopyranoside, 2-propenyl
2-deoxy-3-O-[3-(phenylmethoxy)decyl]-2-[(trifluoroacetyl)amino]-,
6-acetate, (S)- (9CI) (CA INDEX NAME)

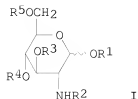
Absolute stereochemistry.



L33 ANSWER 20 OF 42 HCAPLUS COPYRIGHT 2008 ACS on STN

TI Preparation of lipid A monosaccharide analogs as immunostimulants and
antitumor agents.

GI



AB The title compds. [I; one of R1,R4 = H, P(O)(OH)2, protecting group; the other = P(O)(OH)2; one of R2,R3 = (halo-, HO-, or C6-20 aliphatic acyloxy-substituted) C6-20 aliphatic acyl and the other = halo-, HO-, or C6-20 aliphatic acyloxy-substituted C6-20 aliphatic acyl, (halo-, HO-, or C6-20 aliphatic acyloxy-substituted) C6-20 alkyl], possessing macrophage-activating activity (no data), are prepared. Thus, amidation of I (R1 = allyl, R2 = R3 = H, R4R5 = CMe2) (preparation given) with (R)-3-benzoyloxymyristic acid in CH2Cl2 containing DCC followed by esterification with (±)-syn-2-fluoro-3-benzoyloxycarboxyloxymyristic acid in CH2Cl2 containing DCC and 4-dimethylaminopyridine gave I [R1 = allyl, R2 = (R)-Me(CH2)10CH(OCH2Ph)CH2CO, R3 = (±)-Me(CH2)10CH(OCO2CH2Ph)CHFCO, R4R5 = CMe2]. The latter was treated with 1,5-cyclooctadiene-bis[methyldiphenylphosphine]iridium hexafluorophosphate and then H2, iodine, and pyridine to give I (R1 = H; R2-R5 = same as above) which was phosphorylated with (PhCH2O)2P(O)Cl in THF in the presence of BuLi followed by hydrogenolysis over 10% Pd/C to give I [R1 = P(O)(OH)2, R2 = (R)-Me(CH2)10CH(OH)CH2CO, R3 = (±)-Me(CH2)10CH(OH)CHFCO, R4 = R5 = H]. Addnl. 19 I were prepared

AN 1992:59901 HCAPLUS <<LOGINID:20081210>>

DN 116:59901

OREF 116:10385a,10388a

TI Preparation of lipid A monosaccharide analogs as immunostimulants and antitumor agents.

IN Shiosaki, Masao; Ishida, Noboru; Kobayashi, Tomoo; Hiraoka, Tetsuo; Akamatsu, Minoru; Nishijima, Masahiro

PA Sankyo Co., Ltd., Japan

SO Jpn. Kokai Tokkyo Koho, 54 pp.

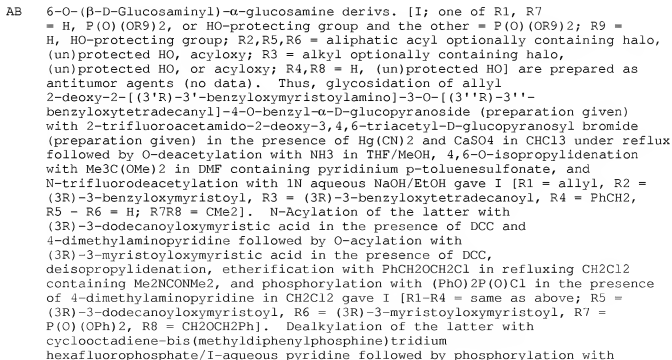
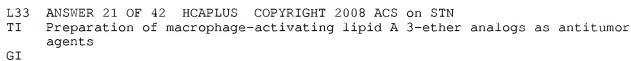
CODEN: JKXXAF

DT Patent

LA Japanese

FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 02256697	A	19901017	JP 1989-321153	19891211 <--
	JP 2839921	B2	19981224		
	DD 295854	A5	19911114	DD 1990-342041	19900625 <--
	SU 1836378	A3	19930823	SU 1990-4830600	19900625 <--
	CN 1052481	A	19910626	CN 1990-106805	19900626 <--
	CN 1029405	C	19950802		
	HU 55793	A2	19910628	HU 1990-3991	19900626 <--
	HU 217114	B	19991129		
	CZ 285583	B6	19990915	CZ 1990-3185	19900626 <--
	CA 2019972	A1	19910611	CA 1990-2019972	19900627 <--
	CA 2019972	C	20000808		
	EP 437016	A2	19910717	EP 1990-307045	19900627 <--
	EP 437016	B1	19960501		
	R: AT, BE, CH, DE, DK, ES, FR, GB, IT, LU, NL, SE				
	AT 137504	T	19960515	AT 1990-307045	19900627 <--
	ES 2088970	T3	19961001	ES 1990-307045	19900627 <--



(PhCH₂O)2P(O)Cl in the presence of BuLi in THF and hydrogenolysis over 10% Pd/C and then PtO₂ in MeOH/THF gave I [R₁ = R₇ = P(O)(OH)₂, R₂ = (3R)-3-hydroxy-myristoyl, R₃ = (3R)-3-hydroxytetradecanoyl, R₄ = R₈ = H, R₅ = (3R)-3-dodecanoyloxymyristoyl, R₆ = (3R)-3-myristoyloxymyristoyl].

AN 1991:632768 HCAPLUS <<LOGINID::20081210>>

DN 115:232768

OREF 115:39701a,39704a

TI Preparation of macrophage-activating lipid A 3-ether analogs as antitumor agents

IN Shiosaki, Masao; Ishida, Noboru; Kobayashi, Tomoo; Hiraoka, Tetsuo; Akamatsu, Minoru; Nishijima, Masahiro

PA Sankyo Co., Ltd., Japan

SO Jpn. Kokai Tokkyo Koho, 26 pp.

CODEN: JKXXAF

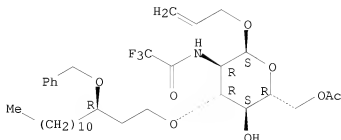
DT Patent

LA Japanese

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 03135990	A	19910610	JP 1989-273524	19891020 <--
	JP 2839916	B2	19981224		
PRAI	JP 1989-273524		19891020	<--	
OS	MARPAT 115:232768				
IT	137014-95-0P 137042-22-9P				
RL:	SPN (Synthetic preparation); PREP (Preparation) (preparation of, as intermediate for antitumor lipid A analog)				
RN	137014-95-0	HCAPLUS			
CN	α -D-Glucopyranoside, 2-propenyl 2-deoxy-3-O-[3-(phenylmethoxy)tetradecyl]-2-[(trifluoroacetyl)amino]-, 6-acetate, (R)- (9CI) (CA INDEX NAME)				

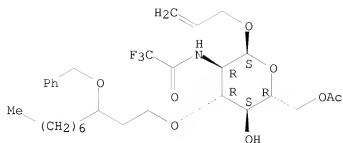
Absolute stereochemistry.



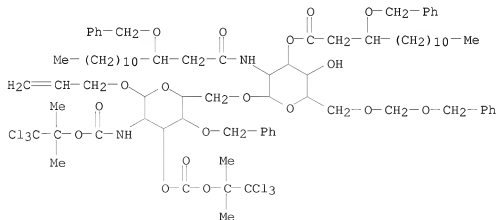
RN 137042-22-9 HCAPLUS

CN α -D-Glucopyranoside, 2-propenyl
2-deoxy-3-O-[3-(phenylmethoxy)decyl]-2-[(trifluoroacetyl)amino]-,
6-acetate (9CI) (CA INDEX NAME)

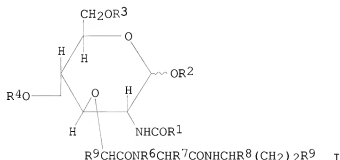
Absolute stereochemistry.



L33 ANSWER 22 OF 42 HCAPLUS COPYRIGHT 2008 ACS on STN
 TI Lipid A and related compounds. XXIV. Efficient synthesis of several lipid as via common disaccharide intermediates
 AB The development of new common disaccharide intermediates bearing 2 amino and 6 hydroxyl groups that are chemical differentiated, and their application to syntheses of several lipids As, is described.
 AN 1991:247631 HCAPLUS <<LOGINID::20081210>>
 DN 114:247631
 OREF 114:41833a,41836a
 TI Lipid A and related compounds. XXIV. Efficient synthesis of several lipid as via common disaccharide intermediates
 AU Akamatsu, Seiji; Ikeda, Kiyoshi; Achiwa, Kazuo
 CS Sch. Pharm. Sci., Univ. Shizuoka, Shizuoka, 422, Japan
 SO Chemical & Pharmaceutical Bulletin (1991), 39(2), 288-96
 CODEN: CPBTAL; ISSN: 0009-2363
 DT Journal
 LA English
 OS CASREACT 114:247631
 IT 134040-50-9P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and phosphitylation of)
 RN 134040-50-9 HCAPLUS
 CN β -D-Glucopyranoside, 2-propenyl 2-deoxy-6-O-[2-deoxy-3-O-[1-oxo-3-(phenylmethoxy)tetradecyl]-2-[[1-oxo-3-(phenylmethoxy)tetradecyl]amino]-6-O-[(phenylmethoxy)methyl]- β -D-glucopyranosyl]-4-O-(phenylmethyl)-2-[[[(2,2,2-trichloro-1,1-dimethylethoxy)carbonyl]amino]-, 3-(2,2,2-trichloro-1,1-dimethylethyl carbonate), [6(2(R),3(R))]- (9CI) (CA INDEX NAME)



L33 ANSWER 23 OF 42 HCAPLUS COPYRIGHT 2008 ACS on STN
 TI Preparation of dipeptidyl-4-O,6-O-acyl-2-amino-2-deoxy-D-glucose
 GI derivatives for use in AIDS-immunocompromised human hosts



AB The title compds. I [R1 = (un)substituted alkyl or Ph, etc.; R2 = H, (un)substituted alkyl, Ph, phenylalkyl, etc.; R3, R4 = R10(CO)rXs(CR11R12)tCO; R5 = H, alkyl; R6 = H, R6R7 = (CH2)3, R7 = H, alkyl, HOCH2, HSCH2, (un)substituted benzyl; R8, R9= CO2H, alkoxy, carbonyl, (un)substituted CONH2, etc.; R10 = H, alkyl, alkenyl, alkoxy, Ph, alkylsulfonyl, cholesteryl; X = O, S, SiR13R14; R11-R14 = H, alkyl, alkylcarbonyloxy, etc.; r, s = 0, 1; t = 0-20] are prepared as drugs for enhancing host resistance against opportunistic infections in AIDS patients. Benzyl-2-acetamido-2-deoxy-3-O-(D-2-propionyl-L-alanyl-D-isoglutamine benzyl ester)-α-D-glucopyranoside was treated successively with DMF, behenoyloxyisobutyric acid, CH2Cl2, N,N'-dicyclohexylcarbodiimide, and 4-dimethylaminopyridine to give benzyl-2-acetamido-6-O-behenoyloxyisobutyl-2-deoxy-3-O-(D-2-propionyl-L-alanyl-D-isoglutamine benzyl ester)-α-D-glucopyranoside, which upon hydrogenolysis over Pd in HOAc gave 2-acetamido-6-O-behenoyloxyisobutyl-2-deoxy-3-O-(D-2-propionyl-L-alanyl-D-isoglutamine)-D-glucose. I, administered s.c. at 100-300 mg/kg/day for 5 consecutive days, increased the production of antibodies against bovine serum albumin in mice (no specific examples).

AN 1990:112075 HCAPLUS <<LOGINID:20081210>>

DN 112:112075

OREF 112:18799a,18802a

TI Preparation of dipeptidyl-4-O,6-O-acyl-2-amino-2-deoxy-D-glucose derivatives for use in AIDS-immunocompromised human hosts

IN Durette, Philippe L.; Dorn, Conrad P.

PA Merck and Co., Inc., USA

SO U.S., 16 pp.

CODEN: USXXAM

DT Patent

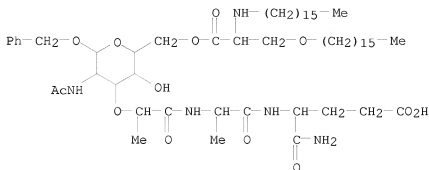
LA English

FAN.CNT 1

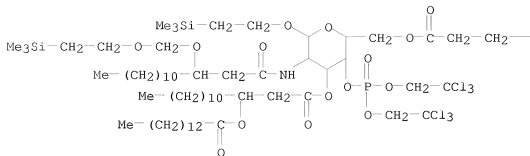
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 4868155	A	19890919	US 1987-105055	19871005 <--
PRAI	US 1987-105055		19871005	<--	
IT	125598-54-1P				

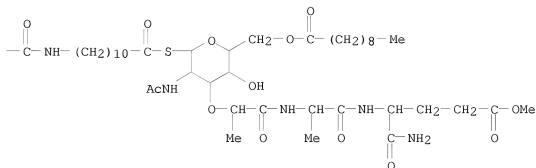
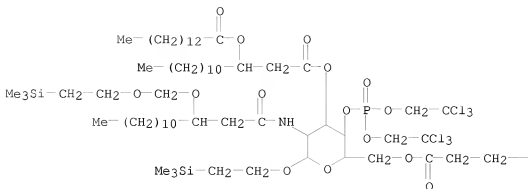
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and hydrogenolysis of)
 RN 125598-54-1 HCAPLUS
 CN D- α -Glutamine, N2-[N-[N-acetyl-1-O-(phenylmethyl)- α -muramoyl]-L-alanyl]-, 6'-ester with N,O-dihexadecylserine (9CI) (CA INDEX NAME)



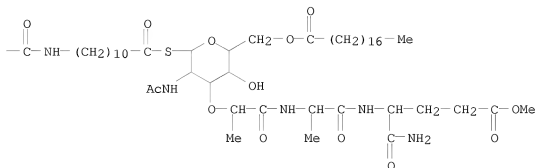
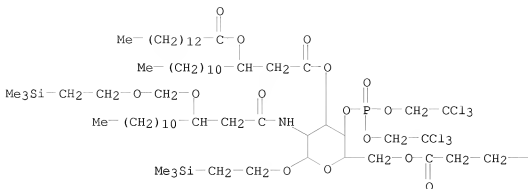
L33 ANSWER 24 OF 42 HCAPLUS COPYRIGHT 2008 ACS on STN
 TI Studies on immunoadjuvant active compounds. Part XXXVII. Synthesis and immunoadjuvant activity of the conjugates of 1-thio-N-acetyl-muramoyl dipeptide with lipid A subunit analogs
 AB A variety of immunomodulators were synthesized by combining biol active derivs. of 1-thio-muramoyl dipeptide with 4-O-phosphono-D-glucosamine derivs. related to bacterial lipid A, and using the (succinoylamino)undecanoyl group as a spacer. Their immunoadjuvant activities in guinea-pigs were examined, and the compds. showed strong delayed type of hypersensitivity to N-acetyl-L-tyrosine-3-azobenzene-4'-arsonate, comparable to that of N-acetylmuramoyl dipeptide.
 AN 1989:566954 HCAPLUS <<LOGINID::20081210>>
 DN 111:166954
 OREF 111:27625a,27628a
 TI Studies on immunoadjuvant active compounds. Part XXXVII. Synthesis and immunoadjuvant activity of the conjugates of 1-thio-N-acetyl-muramoyl dipeptide with lipid A subunit analogs
 AU Ogawa, Yuji; Kitagawa, Masayuki; Fujishima, Yushun; Kiso, Makoto; Hasegawa, Akira; Ishida, Hideharu; Azuma, Ichiro
 CS Dep. Appl. Bioorg. Chem., Gifu Univ., Gifu, 501-11, Japan
 SO Agricultural and Biological Chemistry (1989), 53(4), 1025-36
 CODEN: ABCHA6; ISSN: 0002-1369
 DT Journal
 LA English
 IT 122078-92-6P 122078-93-7P 122078-94-8P
 122099-34-7P 122099-35-8P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and desilylation of)
 RN 122078-92-6 HCAPLUS
 CN D- α -Glutamine, N2-[N-[N-acetyl-1-S-acetyl-6-O-[11-[(3-carboxy-1-oxopropyl)amino]-1-oxoundecyl]-1-thio- β -muramoyl]-L-alanyl]-, 5-methyl ester, 6-ester with [2(R),3(R)]-2-(trimethylsilyl)ethyl 2-deoxy-2-[[1-oxo-3-[[2-(trimethylsilyl)ethoxy]methoxy]tetradecyl]amino]- β -D-glucopyranoside 4-[bis(2,2,2-trichloroethyl) phosphate] 3-[3-[(1-oxotetradecyl)oxy]tetradecanoate] (9CI) (CA INDEX NAME)





RN 122099-35-8 HCAPLUS

CN D- α -Glutamine, N2-[N-[N-acetyl-1-S-[11-[(3-carboxy-1-oxopropyl)amino]-1-oxoundecyl]-6-O-(1-oxooctadecyl)-1-thio- β -muramoyl]-L-alanyl]-, 5-methyl ester, 6-ester with [2(R),3(R)]-2-(trimethylsilyl)ethyl 2-deoxy-2-[[1-oxo-3-[[2-(trimethylsilyl)ethoxy]methoxy]tetradecyl]amino]- β -D-glucopyranoside 4-[bis(2,2,2-trichloroethyl) phosphate] 3-[3-[[1-oxotetradecyl]oxy]tetradecanoate] (9CI) (CA INDEX NAME)



L33 ANSWER 25 OF 42 HCAPLUS COPYRIGHT 2008 ACS on STN

TI Preparation of physiologically active conjugates of lipid A nonreducing monosaccharide subunit analogs with 1-thiomuramyl dipeptide derivatives

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The title conjugates [I; X = O, R = R1 = H; l = 8-12; m = 0-22; n = 1-15; provided that the asym. C's at the 3-position of 2- or 3-substituents in the pyranose ring may have S- or R-configuration], having physiol. activity (no data), were prepared Treatment of I (X = OH, OR = β -OCH2CH2SiMe3, R1 = C13CCH2; l = 12) (II) (preparation given) with DCC

and concentrated H₂SO₄ in 1,4-dioxane and reaction of the active intermediate with 1-thiomuramyl dipeptide derivative QH·CF₃CO₂H (m = 0, n = 10) in MeOH/1,4-dioxane containing Et₃N gave 42.2% I (X = Q, OR = β-OCH₂CH₂SiMe₃, R₁ = CCl₃CH₂, l = 12, m = 0, n = 10). Deprotection of the latter by treatment with BF₃·OEt₂ in Cl₂H₂ to remove Me₃SiCH₂CH₂, followed by Zn powder to remove Cl₃CCCH₂ in AcOH, gave I (X = Q, R = R₁ = H, l = 12, m = 0, n = 10).

AN 1989:515701 HCAPLUS <<LOGINID:20081210>>

DN 111:115701

OREF 111:19407a,19410a

TI Preparation of physiologically active congenates of lipid A nonreducing monosaccharide subunit analogs with 1-thiomuramyl dipeptide derivatives

IN Hasegawa, Akira; Kiso, Makoto; Morihara, Kazuyuki

PA Toho Pharmaceutical Industries Co., Ltd., Japan

SO Jpn. Kokai Tokkyo Koho, 6 pp.

CODEN: JKXXAF

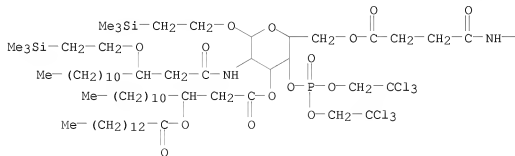
DT Patent

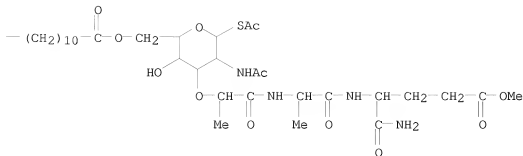
LA Japanese

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 01019098	A	19890123	JP 1987-175766	19870714 <--
PRAI	JP 1987-175766		19870714	<--	
OS	MARPAT 111:115701				
IT	122266-80-2P				
	RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)				
	(preparation and deprotection of)				
RN	122266-80-2 HCAPLUS				
CN	D-α-Glutamine, N2-[N-[N-acetyl-1-S-acetyl-6-O-[11-[(3-carboxy-1-oxopropyl)amino]-1-oxoundecyl]-1-thio-β-muramoyl]-L-alanyl]-, 1-methyl ester, 6-ester with 2-(trimethylsilyl)ethyl 2-deoxy-2-[[1-oxo-3-[2-(trimethylsilyl)ethoxy]tetradecyl]amino]-β-D-glucopyranoside 4-[bis(2,2,2-trichloroethyl) phosphate] 3-[3-[(1-oxotetradecyl)oxy]tetradecanoate], [R-(R*,R*)]- (9CI) (CA INDEX NAME)				

PAGE 1-A





L33 ANSWER 26 OF 42 HCAPLUS COPYRIGHT 2008 ACS on STN

TI Preparation of six naturally occurring sialic acids with immobilized acylneuraminase pyruvate lyase

AB Acylneuraminase pyruvate lyase immobilized on agarose was stable for several months at 4° in buffer, and the same sample could be used up to ten times in the preparation of sialic acids from the corresponding mannosamines and pyruvate. Six naturally occurring sialic acids, Neu5Ac, Neu5Ac2, Neu5Ac9Lac, Neu5Gc, Neu9Ac5Gc and the 2-acetoxyacetamido derivative were thus obtained, in multigram quantities when needed. 2-Acetamido-2-deoxy-5-O-methyl-D-mannose gave only traces of Neu5Ac8Me, one of the starfish sialic acids, but other methylated derivs., Neu5Ac7Me and Neu5Ac9Me were readily obtained. This indicated a specific sensitivity of the enzyme to 8-O-substitution on sialic acid or 5-O-substitution on N-acetylmannosamine. Also reported are inexpensive chemical routes to the substrates, which avoid the use of costly mannosamine as starting material.

AN 1989:423846 HCAPLUS <<LOGINID:20081210>>

DN 111:23846

OREF 111:4165a, 4168a

TI Preparation of six naturally occurring sialic acids with immobilized acylneuraminase pyruvate lyase

AU Auge, Claudine; David, Serge; Gautheron, Christine; Malleron, Annie; Cavaye, Bertrand

CS Inst. Chim. Mol., Univ. Paris Sud, Orsay, 91405, Fr.

SO New Journal of Chemistry (1988), 12(8-9), 733-44

CODEN: NJCHE5; ISSN: 1144-0546

DT Journal

LA English

OS CASREACT 111:23846

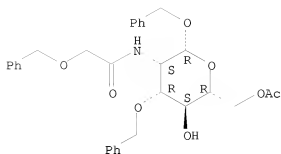
IT 119870-61-0P 119887-65-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and hydrogenolysis of)

RN 119870-61-0 HCAPLUS

CN β-D-Mannopyranoside, phenylmethyl 2-deoxy-2-[(phenylmethoxy)acetyl]amino]-3-O-(phenylmethyl)-, 6-acetate (9CI) (CA INDEX NAME)

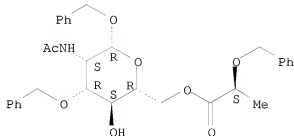
Absolute stereochemistry.



RN 119887-65-9 HCAPLUS

CN β -D-Mannopyranoside, phenylmethyl
2-(acetylamino)-2-deoxy-3-O-(phenylmethyl)-,
6-[2-(phenylmethoxy)propanoate], (S)- (9CI) (CA INDEX NAME)

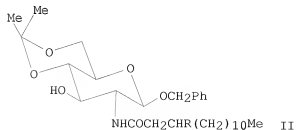
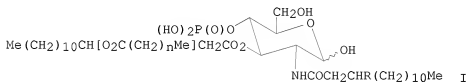
Absolute stereochemistry.



L33 ANSWER 27 OF 42 HCAPLUS COPYRIGHT 2008 ACS on STN

TI Nonreducing sugar subunit analogs of bacterial lipid A carrying the ester
bound (3R)-3-(acyloxy)tetradecanoyl group

GI



AB In order to elucidate further the relationship between the composition of the fatty acyl groups in the nonreducing-sugar subunit of bacterial lipid A and its biol. activity, analogs (R,R)-I (n = 10, 14, R = OH) and (R)-I (n = 10, 12, 14, R = H) have been synthesized. Isopropylidene- β -D-glucopyranosides II (R = H, OCH₂OCH₂Ph) were each esterified with (3R)-Me(CH₂)₁₀CH[O₂C(CH₂n)Me]CH₂CO₂H followed by deisopropylidenation, 6-O-tritylation and 4-O-phosphorylation, to give I.

AN 1988:631430 HCAPLUS <<LOGINID:20081210>>

DN 109:231430

OREF 109:38297a,38300a

TI Nonreducing sugar subunit analogs of bacterial lipid A carrying the ester bound (3R)-3-(acyloxy)tetradecanoyl group

AU Kiso, Makoto; Ogawa, Yuji; Fujishima, Yushun; Fujita, Minoru; Tanaka, Shinji; Hasegawa, Akira

CS Dep. Agric. Chem., Gifu Univ., Gifu, 501-11, Japan

SO Journal of Carbohydrate Chemistry (1987), 6(4), 625-38
CODEN: JCACDM; ISSN: 0732-8303

DT Journal

LA English

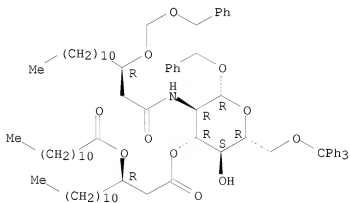
OS CASREACT 109:231430

IT 117639-30-2P 117639-33-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and phosphorylation of)

RN 117639-30-2 HCAPLUS

CN β -D-Glucopyranoside, phenylmethyl 2-deoxy-2-[[1-oxo-3-[(phenylmethoxy)methoxy]tetradecyl]amino]-6-O-(triphenylmethyl)-, 3-[3-[(1-oxododecyl)oxy]tetradecanoate], [2(R),3(R)]-(9CI) (CA INDEX NAME)

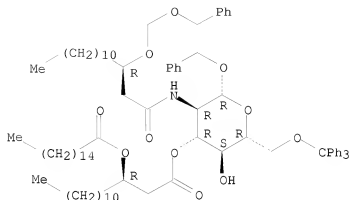
Absolute stereochemistry.



RN 117639-33-5 HCAPLUS

CN β -D-Glucopyranoside, phenylmethyl 2-deoxy-2-[[1-oxo-3-[(phenylmethoxy)methoxy]tetradecyl]amino]-6-O-(triphenylmethyl)-, 3-[3-[(1-oxohexadecyl)oxy]tetradecanoate], [2(R),3(R)]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



L33 ANSWER 28 OF 42 HCAPLUS COPYRIGHT 2008 ACS on STN

TI Total synthesis of Escherichia coli lipid A, the endotoxically active principle of cell-surface lipopolysaccharide

GI For diagram(s), see printed CA Issue.

AB Chemical syntheses are described of polyacylated $\beta(1\rightarrow6)$ glucosamine disaccharide 1,4'-diphosphates I [R = R4 = P(O)(OH)2; throughout the abstract R1 = (R)-3-(tetradecanoyloxy)tetradecanoyl, R2 = (R)-3-(dodecanoyloxy)tetradecanoyl, R3 = (R)-3-hydroxytetradecanoyl; II], which correspond to the proposed structure of E. coli lipid A, and of their dephospho derivs. [I; R = P(O)(OH)2, R4 = H; R = H, R4 = P(O)(OH)2; R = R4 = H]. II proved to be identical with the natural specimen. The chemical structure of lipid A was thus established.

AN 1988:204945 HCAPLUS <<LOGINID::20081210>>

DN 108:204945

OREF 108:33693a,33696a

TI Total synthesis of Escherichia coli lipid A, the endotoxically active principle of cell-surface lipopolysaccharide

AU Imoto, Mashiro; Yoshimura, Hiroyuki; Shimamoto, Tetsuo; Sakaguchi, Nobuki; Kusumoto, Shoichi; Shiba, Tetsuo

CS Fac. Sci., Osaka Univ., Toyonaka, 560, Japan

SO Bulletin of the Chemical Society of Japan (1987), 60(6), 2205-14

CODEN: BCSJA8; ISSN: 0009-2673

DT Journal

LA English

OS CASREACT 108:204945

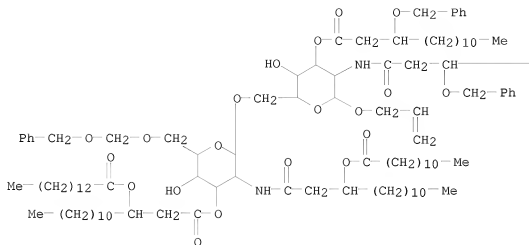
IT 114360-75-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and deacylation of)

RN 114360-75-7 HCAPLUS

CN α -D-Glucopyranoside, 2-propenyl

2-deoxy-6-O-[2-deoxy-2-[[1-oxo-3-[(1-oxododecyl)oxy]tetradecyl]amino]-3-O-[1-oxo-3-[(1-oxotetradecyl)oxy]tetradecyl]-6-O-[(phenylmethoxy)methyl]- β -D-glucopyranosyl]-2-[[1-oxo-3-(phenylmethoxy)tetradecyl]amino]-, 3-[3-(phenylmethoxy)tetradecanoate], [2(R),3(R),6[2(R),3(R)]]- (9CI) (CA INDEX NAME)



— (CH₂)₁₀—Me

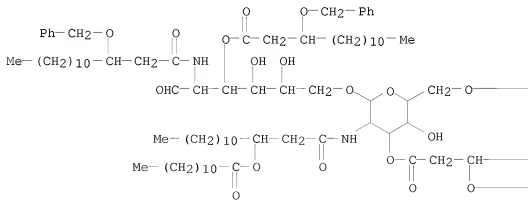
IT 114360-76-8P

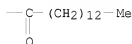
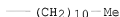
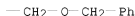
RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation and phosphorylation of, with dibenzyl phosphorochloridate)

RN 114360-76-8 HCAPLUS

CN D-Glucose, 2-deoxy-6-O-[2-deoxy-2-[[1-oxo-3-[(1-oxododecyl)oxy]tetradecyl]amino]-3-O-[1-oxo-3-[(1-oxotetradecyl)oxy]tetradecyl]-6-O-[(phenylmethoxy)methyl]-β-D-glucopyranosyl]-2-[[1-oxo-3-(phenylmethoxy)tetradecyl]amino]-, 3-[3-(phenylmethoxy)tetradecanoate], [2(R),3(R),6[2(R),3(R)]]- (9CI) (CA INDEX NAME)

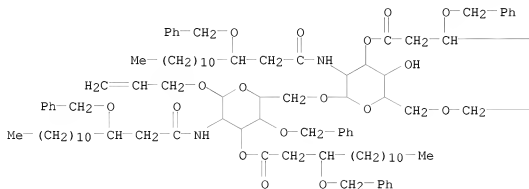




L33 ANSWER 29 OF 42 HCAPLUS COPYRIGHT 2008 ACS on STN
 TI Chemical synthesis of a biosynthetic precursor of lipid A with a
 phosphorylated tetraacyl disaccharide structure
 GI For diagram(s), see printed CA Issue.
 AB Glucosamine disaccharide diphosphate [I; R = (R)-3-hydroxytetradecanoyl
 throughout; R1 = R2 = P(O)(OH)2] was prepared via preparation of the
 β -(1 \rightarrow 6)-disaccharide without long chain acyl groups,
 introduction of 3-(benzyloxy)tetradecanoyl groups onto the 2 amino and 2
 OH groups, phosphorylation of the 4'-position, phosphorylation of the
 glycosidic position, and hydrogenolytic deprotection. The monophosphates
 I [R1 = P(O)(OH)2, R2 = H; R1 = H, R2 = P(O)(OH)2] and the dephospho
 derivative I (R1 = R2 = H) were prepared by slight modification of the above
 synthetic route. The diphosphate prepared was identical with a natural
 biosynthetic precursor of lipid A which corresponds to the lipophilic part
 of the lipopolysaccharide (LPS) in the bacterial cell wall. The synthetic
 di- and monophosphates exhibited many of the typical endotoxic activities
 of LPS. This established the chemical structure of the biosynthetic
 precursor of lipid A and elucidated the fundamental structure required for
 the expression of these activities.
 AN 1988:204944 HCAPLUS <<LOGINID:20081210>>
 DN 108:204944
 OREF 108:33693a,33696a
 TI Chemical synthesis of a biosynthetic precursor of lipid A with a
 phosphorylated tetraacyl disaccharide structure
 AU Imoto, Masahiro; Yoshimura, Hiroyuki; Yamamoto, Michiharu; Shimamoto,
 Tetsuo; Kusumoto, Shoichi; Shiba, Tetsuo
 CS Fac. Sci., Osaka Univ., Toyonaka, 560, Japan
 SO Bulletin of the Chemical Society of Japan (1987), 60(6),
 2197-204
 CODEN: BCSJA8; ISSN: 0009-2673
 DT Journal
 LA English
 OS CASREACT 108:204944
 IT 92949-59-2P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation and phosphorylation of, with di-Ph phosphorochloridate)
 RN 92949-59-2 HCAPLUS

CN β -D-Glucopyranoside, 2-propenyl
 2-deoxy-6-O-[2-deoxy-3-O-[1-oxo-3-(phenylmethoxy)tetradecyl]-2-[[1-oxo-3-(phenylmethoxy)tetradecyl]amino]-6-O-[(phenylmethoxy)methyl]- β -D-glucopyranosyl]-2-[[1-oxo-3-(phenylmethoxy)tetradecyl]amino]-4-O-(phenylmethyl)-, 3-[3-(phenylmethoxy)tetradecanoate],
 [2(R),3(R),6[2(R),3(R)]]- (9CI) (CA INDEX NAME)

PAGE 1-A

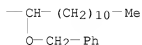
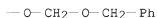
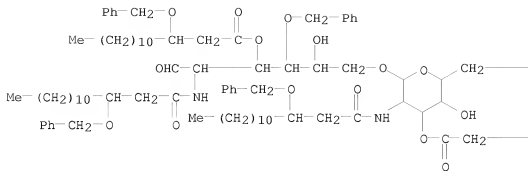


PAGE 1-B

— (CH₂)₁₀—Me

——— O—CH₂—Ph

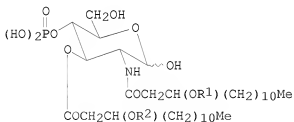
IT 92949-60-5P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation and phosphorylation of, with dibenzyl phosphorochloridate)
 RN 92949-60-5 HCAPLUS
 CN D-Glucose, 2-deoxy-6-O-[2-deoxy-3-O-[1-oxo-3-(phenylmethoxy)tetradecyl]-2-[[1-oxo-3-(phenylmethoxy)tetradecyl]amino]-6-O-[(phenylmethoxy)methyl]- β -D-glucopyranosyl]-2-[[1-oxo-3-(phenylmethoxy)tetradecyl]amino]-4-O-(phenylmethyl)-, 3-[3-(phenylmethoxy)tetradecanoate],
 [2(R),3(R),6[2(R),3(R)]]- (9CI) (CA INDEX NAME)



L33 ANSWER 30 OF 42 HCAPLUS COPYRIGHT 2008 ACS on STN

TI Synthesis of the optically active 4-O-phosphono-D-glucosamine derivatives related to the nonreducing sugar subunit of bacterial lipid A

GI



I

AB The optically active lipid A-subunit homologs named GLA-46, GLA-47, GLA-59, and GLA-60 [I; R1 = R2 = H; R1 = R2 = myristoyl; R1 = myristoyl, R2 = H; R1 = H, R2 = myristoyl; resp.] were prepared stepwise by successive acylation at N-2 and O-3 of benzyl

2-amino-2-deoxy-4,6-O-isopropylidene-β-D-glucopyranoside with the 3-O-(benzyloxy)methyl or 3-O-tetradecanoyl derivative of optically active 3-hydroxytetradecanoic acid, and phosphorylation at O-4 of the D-glucosamine residue.

AN 1988:75749 HCAPLUS <<LOGINID::20081210>>

DN 108:75749

OREF 108:12551a,12554a

TI Synthesis of the optically active 4-O-phosphono-D-glucosamine derivatives related to the nonreducing sugar subunit of bacterial lipid A

AU Kiso, Makoto; Tanaka, Shinji; Fujita, Minoru; Fujishima, Yushun; Ogawa, Yuji; Ishida, Hideharu; Hasegawa, Akira

CS Dep. Agric. Chem., Gifu Univ., Gifu, 501-11, Japan

SO Carbohydrate Research (1987), 162(1), 127-40

CODEN: CRBRAT; ISSN: 0008-6215

DT Journal

LA English

OS CASREACT 108:75749

IT 111247-18-8P 111247-27-9P 112475-24-8P

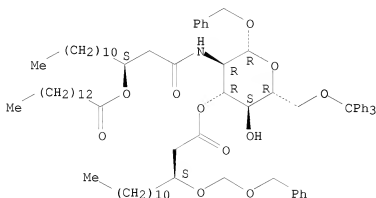
112475-28-2P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and phosphorylation of)

RN 111247-18-8 HCAPLUS

CN β-D-Glucopyranoside, phenylmethyl
2-deoxy-2-[[1-oxo-3-[(1-oxotetradecyl)oxy]tetradecyl]amino]-6-O-
(triphenylmethyl)-, 3-[3-[(phenylmethoxy)methoxy]tetradecanoate],
[2(S),3(S)]- (9CI) (CA INDEX NAME)

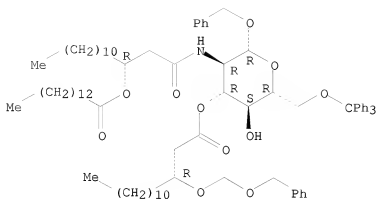
Absolute stereochemistry.



RN 111247-27-9 HCAPLUS

CN β-D-Glucopyranoside, phenylmethyl
2-deoxy-2-[[1-oxo-3-[(1-oxotetradecyl)oxy]tetradecyl]amino]-6-O-
(triphenylmethyl)-, 3-[3-[(phenylmethoxy)methoxy]tetradecanoate],
[2(R),3(R)]- (9CI) (CA INDEX NAME)

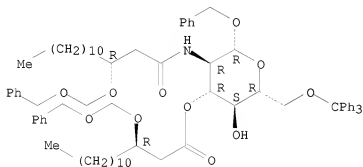
Absolute stereochemistry.



RN 112475-24-8 HCAPLUS

CN β -D-Glucopyranoside, phenylmethyl
2-deoxy-2-[[1-oxo-3-[(phenylmethoxy)methoxy]tetradecyl]amino]-6-O-
(triphenylmethyl)-, 3-[3-[(phenylmethoxy)methoxy]tetradecanoate],
[2(R),3(R)]- (9CI) (CA INDEX NAME)

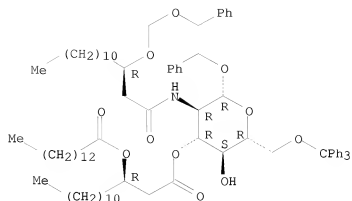
Absolute stereochemistry.



RN 112475-28-2 HCAPLUS

CN β -D-Glucopyranoside, phenylmethyl
2-deoxy-2-[[1-oxo-3-[(phenylmethoxy)methoxy]tetradecyl]amino]-6-O-
(triphenylmethyl)-, 3-[3-[(1-oxotetradecyl)oxy]tetradecanoate],
[2(R),3(R)]- (9CI) (CA INDEX NAME)

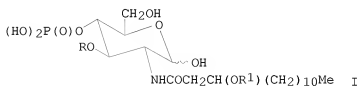
Absolute stereochemistry.



L33 ANSWER 31 OF 42 HCAPLUS COPYRIGHT 2008 ACS on STN

TI Synthesis of the nonreducing-sugar subunit analogs of bacterial lipid A carrying the amide-bound (3R)-3-(acyloxy)tetradecanoyl group

GI



AB Two types of the optically active, 4-O-phosphono-D-glucosamine derivs. related to the nonreducing-sugar subunit of bacterial lipid A, one being GLA-57 [I; R = Me(CH₂)₁₂CO, R₁ = Me(CH₂)₁₀CO] and GLA-58 [I; R = Me(CH₂)₁₂CO, R₁ = Me(CH₂)₁₄CO], and the other GLA-61 [I; R = Me(CH₂)₁₀CH(OH)CH₂CO, R₁ = Me(CH₂)₁₀CO] and GLA-62 [I; R = Me(CH₂)₁₀CH(OH)CH₂CO, R₁ = Me(CH₂)₁₄CO] were prepared. The NH₂ group of benzyl 2-amino-2-deoxy-4,6-O-isopropylidene-β-D-glucopyranoside was first acylated with the (3R)-3-dodecanoyloxytetradecanoyl or (3R)-3-hexadecanoyloxytetradecanoyl group, and then the remaining HO group was esterified with the tetradecanoyl or (3R)-3-(benzyloxymethoxy)tetradecanoyl group, resp. The resulting protected intermediates were each converted, by the sequence of O-deisopropylidenation, 6-O-tritylation, and 4-O-phosphorylation, into I.

AN 1988:38248 HCAPLUS <<LOGINID::20081210>>

DN 108:38248

OREF 108:6415a,6418a

TI Synthesis of the nonreducing-sugar subunit analogs of bacterial lipid A carrying the amide-bound (3R)-3-(acyloxy)tetradecanoyl group

AU Kiso, Makoto; Tanaka, Shinji; Fujita, Minoru; Fujishima, Yushun; Ogawa, Yuji; Hasegawa, Akira

CS Dep. Agric. Chem., Gifu Univ., Gifu, 501-11, Japan

SO Carbohydrate Research (1987), 162(2), 247-56

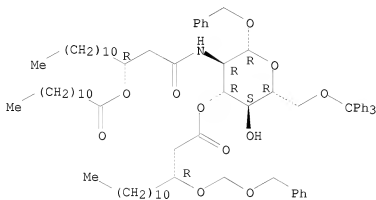
CODEN: CRBRAT; ISSN: 0008-6215

DT Journal

LA English

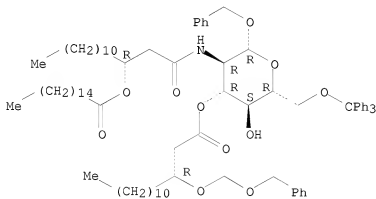
OS CASREACT 108:38248
 IT 112166-26-4P 112166-29-7P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation, phosphorylation and detritylation of)
 RN 112166-26-4 HCAPLUS
 CN β -D-Glucopyranoside, phenylmethyl
 2-deoxy-2-[[1-oxo-3-[(1-oxododecyl)oxy]tetradecyl]amino]-6-O-
 (triphenylmethyl)-, 3-[3-[(phenylmethoxy)methoxy]tetradecanoate],
 [2(R),3(R)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

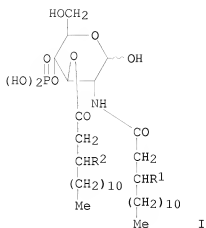


RN 112166-29-7 HCAPLUS
 CN β -D-Glucopyranoside, phenylmethyl
 2-deoxy-2-[[1-oxo-3-[(1-oxohexadecyl)oxy]tetradecyl]amino]-6-O-
 (triphenylmethyl)-, 3-[3-[(phenylmethoxy)methoxy]tetradecanoate],
 [2(R),3(R)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L33 ANSWER 32 OF 42 HCAPLUS COPYRIGHT 2008 ACS on STN
 TI Preparation of biologically active analogs of the nonreducing
 monosaccharide moiety of lipid A
 GI



AB The title glucosamine derivs. [I; R1 = H, OH, O2C(CH2)12Me; R2 = OH, O2C(CH2)12Me], which exhibit higher biol. and immunol. activities than natural lipid A and are useful as mitogens and immunol. adjuvants, were prepared N- And O-acylation of benzyl 2-amino-2-deoxy-4,6-isopropylidene-β-D-glucopyranoside with (3R)-3-(tetradecanoyloxy)tetradecanoic acid was conducted stepwise, first in the presence of 1,3-dicyclohexyldiimide (DCC) and second using DCC and 4-(dimethylamino)pyridine (DMAP) to give benzyl 2-deoxy-2-[(3R)-3-(tetradecanoyloxy)tetradecanamido]-3-O-[(3R)-3-(tetradecanoyloxy)tetradecanoyl]-β-D-glucopyranoside which was subjected to deacetonation in 80% aqueous AcOH, 6-O-tritylation by trityl chloride, esterification with (PhO)2P(O)OH in the presence of DMAP in pyridine, detritylation with HBF4 followed by successive hydrogenolysis over Pd black and PtO2 to give I [R1 = R2 = 3(R)-3-tetradecanoyl].

AN 1987:637220 HCAPLUS <<LOGINID:20081210>>

DN 107:237220

OREF 107:38133a,38136a

TI Preparation of biologically active analogs of the nonreducing monosaccharide moiety of lipid A

IN Hasegawa, Akira; Kiso, Makoto; Morihara, Kazuyuki

PA Toho Pharmaceutical Industries Co., Ltd., Japan

SO Eur. Pat. Appl., 11 pp.

CODEN: EPXXDW

DT Patent

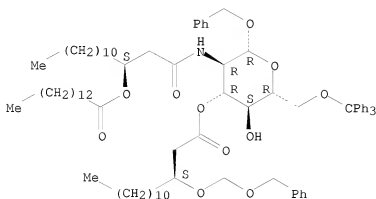
LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 224260	A2	19870603	EP 1986-116474	19861127 <--
	EP 224260	A3	19880406		
	R: CH, DE, FR, GB, IT, LI, NL, SE				
	JP 62129292	A	19870611	JP 1985-268802	19851128 <--
	JP 63030495	A	19880209	JP 1986-174436	19860724 <--
	JP 63044588	A	19880225	JP 1986-188215	19860811 <--
	US 4746742	A	19880524	US 1986-930361	19861112 <--
PRAI	JP 1985-268802	A	19851128	<--	
	JP 1986-174436	A	19860724	<--	
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OS	CASREACT 107:237220; MARPAT 107:237220				

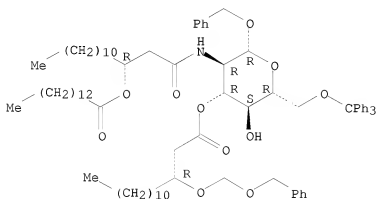
IT 111247-18-8P 111247-27-9P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation and phosphorylation of)
 RN 111247-18-8 HCAPLUS
 CN β -D-Glucopyranoside, phenylmethyl
 2-deoxy-2-[[1-oxo-3-[(1-oxotetradecyl)oxy]tetradecyl]amino]-6-O-
 (triphenylmethyl)-, 3-[3-[(phenylmethoxy)methoxy]tetradecanoate],
 [2(S),3(S)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 111247-27-9 HCAPLUS
 CN β -D-Glucopyranoside, phenylmethyl
 2-deoxy-2-[[1-oxo-3-[(1-oxotetradecyl)oxy]tetradecyl]amino]-6-O-
 (triphenylmethyl)-, 3-[3-[(phenylmethoxy)methoxy]tetradecanoate],
 [2(R),3(R)]- (9CI) (CA INDEX NAME)

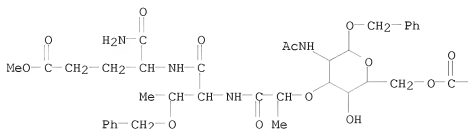
Absolute stereochemistry.



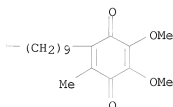
L33 ANSWER 33 OF 42 HCAPLUS COPYRIGHT 2008 ACS on STN
 TI Synthesis and the adjuvant and tumor-suppressive activities of quinonyl
 muramyl dipeptides
 GI

RN 77290-27-8 HCAPLUS
 CN D- α -Glutamine, N2-[N-[N-acetyl-6-O-[10-(4,5-dimethoxy-2-methyl-3,6-dioxo-1,4-cyclohexadien-1-yl)-1-oxodecyl]-1-O-(phenylmethyl)- α -muramoyl]-O-(phenylmethyl)-L-threonyl]-, methyl ester (9CI) (CA INDEX NAME)

PAGE 1-A



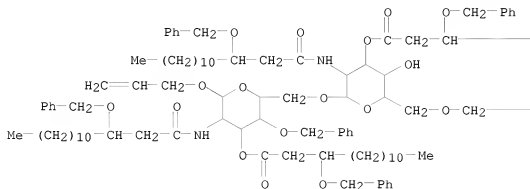
PAGE 1-B



L33 ANSWER 34 OF 42 HCAPLUS COPYRIGHT 2008 ACS on STN
 TI Chemical synthesis of phosphorylated tetraacetyl disaccharide corresponding to a biosynthetic precursor of lipid A
 GI For diagram(s), see printed CA Issue.
 AB A total synthesis of glucosamine disaccharide 1,4'-diphosphate I [RCO = Me(CH₂)₁₀CH(OH)CH₂CO] is described. This is the 1st confirmation of the fundamental structure of lipid A since the synthetic compound exhibited most of the characteristic biol. activities of natural endotoxin.
 AN 1984:611613 HCAPLUS <<LOGINID:20081210>>
 DN 101:211613
 OREF 101:32079a,32082a
 TI Chemical synthesis of phosphorylated tetraacetyl disaccharide corresponding to a biosynthetic precursor of lipid A
 AU Imoto, M.; Yoshimura, H.; Yamamoto, M.; Shimamoto, T.; Kusumoto, S.; Shiba, T.
 CS Fac. Sci., Osaka Univ., Toyonaka, 560, Japan
 SO Tetrahedron Letters (1984), 25(25), 2667-70
 CODEN: TELEAY; ISSN: 0040-4039
 DT Journal
 LA English
 IT 92949-59-2P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and deallylation of)
 RN 92949-59-2 HCAPLUS

CN β -D-Glucopyranoside, 2-propenyl
 2-deoxy-6-O-[2-deoxy-3-O-[1-oxo-3-(phenylmethoxy)tetradecyl]-2-[[1-oxo-3-(phenylmethoxy)tetradecyl]amino]-6-O-[(phenylmethoxy)methyl]- β -D-glucopyranosyl]-2-[[1-oxo-3-(phenylmethoxy)tetradecyl]amino]-4-O-(phenylmethyl)-, 3-[3-(phenylmethoxy)tetradecanoate],
 [2(R),3(R),6[2(R),3(R)]]- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B

— (CH₂)₁₀—Me

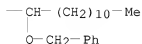
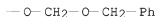
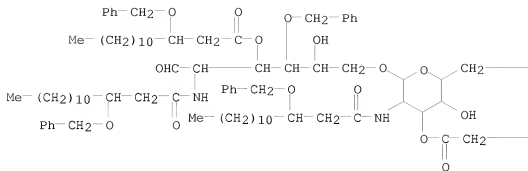
——— O—CH₂—Ph

IT 92949-60-5P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation and phosphorylation of)

RN 92949-60-5 HCAPLUS

CN D-Glucose, 2-deoxy-6-O-[2-deoxy-3-O-[1-oxo-3-(phenylmethoxy)tetradecyl]-2-[[1-oxo-3-(phenylmethoxy)tetradecyl]amino]-6-O-[(phenylmethoxy)methyl]- β -D-glucopyranosyl]-2-[[1-oxo-3-(phenylmethoxy)tetradecyl]amino]-4-O-(phenylmethyl)-, 3-[3-(phenylmethoxy)tetradecanoate],
 [2(R),3(R),6[2(R),3(R)]]- (9CI) (CA INDEX NAME)



L33 ANSWER 35 OF 42 HCAPLUS COPYRIGHT 2008 ACS on STN
 TI Disaccharides
 GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Disaccharides I (R1CO = fatty acid acyl group, R2CO = fatty acid acyl group, R3,R4 = H or phosphate group), useful as mitogens for stimulation of mouse lymphocytes, were prepared. Thus, disaccharide II was converted in 6 steps to III [R1CO = tetradecanoyl, R2CO = 3-(R)-(benzyloxy)tetradecanoyl] which was deprotected and phosphorylated to give I (R1CO = tetradecanoyl, R2CO = 3-hydroxytetradecanoyl, R3 = H, R4 = dihydrogen phosphate). The latter stimulated cultured mouse lymphocytes 2.0 ± 0.2 at $100 \mu\text{g/mL}$.

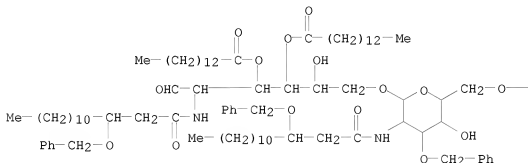
AN 1984:571657 HCAPLUS <<LOGINID:20081210>>
 DN 101:171657
 OREF 101:25975a,25978a
 TI Disaccharides
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 SO Jpn. Kokai Tokkyo Koho, 5 pp.
 CODEN: JKXXAF
 DT Patent

LA Japanese

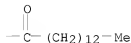
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 59048497	A	19840319	JP 1982-159174	19820913 <--
	JP 02011597	B	19900314		
PRAI	JP 1982-159174		19820913	<--	
IT	88862-35-5P				
	RL: SPN (Synthetic preparation); PREP (Preparation) (preparation and removal of benzyloxy groups from)				
RN	88862-35-5	HCAPLUS			
CN	D-Glucose, 2-deoxy-6-O-[2-deoxy-2-[[1-oxo-3-(phenylmethoxy)tetradecyl]amino]-6-O-(1-oxotetradecyl)-3-O-(phenylmethyl)-β-D-glucopyranosyl]-2-[[1-oxo-3-(phenylmethoxy)tetradecyl]amino]-, 3,4-ditetradecanoate, [2(R),6(R)]- (9CI) (CA INDEX NAME)				

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PAGE 1-B

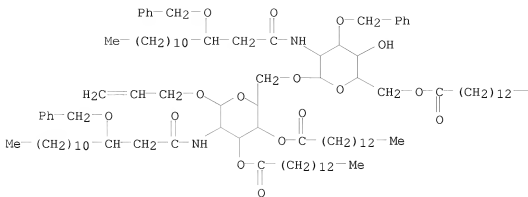


IT 88862-34-4P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 88862-34-4 HCAPLUS

CN β-D-Glucopyranoside, 2-propenyl
2-deoxy-6-O-[2-deoxy-2-[[1-oxo-3-(phenylmethoxy)tetradecyl]amino]-6-O-(1-oxotetradecyl)-3-O-(phenylmethyl)-β-D-glucopyranosyl]-2-[[1-oxo-3-(phenylmethoxy)tetradecyl]amino]-, 3,4-ditetradecanoate, [2(R),6(R)]- (9CI) (CA INDEX NAME)

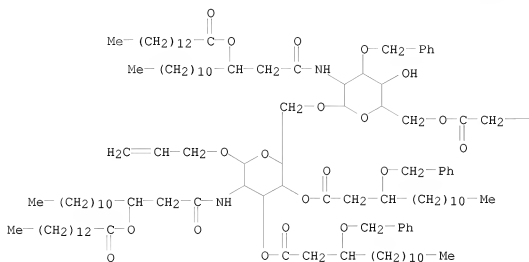


— Me

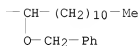
L33 ANSWER 36 OF 42 HCAPLUS COPYRIGHT 2008 ACS on STN
 TI Chemical synthesis of lipid A for the elucidation of structure-activity relationships
 AB A synthetic route for the preparation of an O,N-polyacyl glucosamine β -(1-6)-disaccharide 1,4'-diphosphate, which corresponds to the proposed structure of Salmonella-type lipid A, was developed. Many structural analogs were prepared in order to elucidate the structural requirements for the biol. activities of lipid A.
 AN 1984:121491 HCAPLUS <<LOGINID::20081210>>
 DN 100:121491
 OREF 100:18505a,18508a
 TI Chemical synthesis of lipid A for the elucidation of structure-activity relationships
 AU Kusumoto, S.; Inage, M.; Chaki, H.; Imoto, M.; Shimamoto, T.; Shiba, T.
 CS Fac. Sci., Osaka Univ., Toyonaka, 560, Japan
 SO ACS Symposium Series (1983), 231(Bact. Lipopolysaccharides), 237-54
 CODEN: ACSMC8; ISSN: 0097-6156
 DT Journal
 LA English
 IT 87357-77-5P 88862-34-4P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and deallylation of)
 RN 87357-77-5 HCAPLUS
 CN β -D-Glucopyranoside, 2-propenyl
 2-deoxy-6-O-[2-deoxy-6-O-[1-oxo-3-(phenylmethoxy)tetradecyl]-2-[[1-oxo-3-[(1-oxotetradecyl)oxy]tetradecyl]amino]-3-O-(phenylmethyl)- β -D-glucopyranosyl]-2-[[1-oxo-3-[(1-oxotetradecyl)oxy]tetradecyl]amino]-, 3,4-bis[3-(phenylmethoxy)tetradecanoate], [2(R),3(R),4(R),6[2(R),6(R)]]-

(9CI) (CA INDEX NAME)

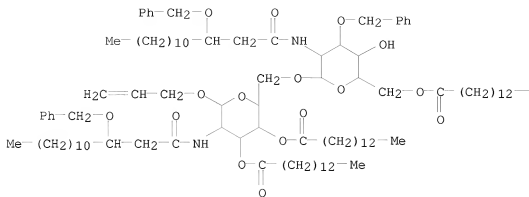
PAGE 1-A



PAGE 1-B

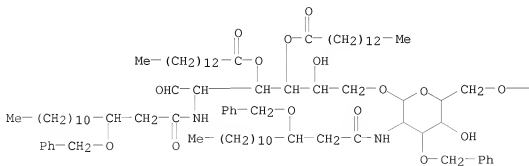


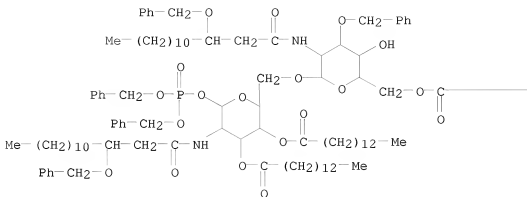
RN 88862-34-4 HCAPLUS
 CN β -D-Glucopyranoside, 2-propenyl
 2-deoxy-6-O-[2-deoxy-2-[[1-oxo-3-(phenylmethoxy)tetradecyl]amino]-6-O-(1-oxotetradecyl)-3-O-(phenylmethyl)- β -D-glucopyranosyl]-2-[[1-oxo-3-(phenylmethoxy)tetradecyl]amino]-, 3,4-ditetradecanoate, [2(R),6(R)]-(9CI) (CA INDEX NAME)



— Me

IT 88862-35-5P 88862-46-8P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation and debenzoylation of)
 RN 88862-35-5 HCAPLUS
 CN D-Glucose, 2-deoxy-6-O-[2-deoxy-2-[[1-oxo-3-(
 phenylmethoxy)tetradecyl]amino]-6-O-(1-oxotetradecyl)-3-O-(phenylmethyl)-
 β-D-glucopyranosyl]-2-[[1-oxo-3-(phenylmethoxy)tetradecyl]amino]-,
 3,4-ditetradecanoate, [2(R),6(R)]- (9CI) (CA INDEX NAME)




$$-(\text{CH}_2)_{12}-\text{Me}$$

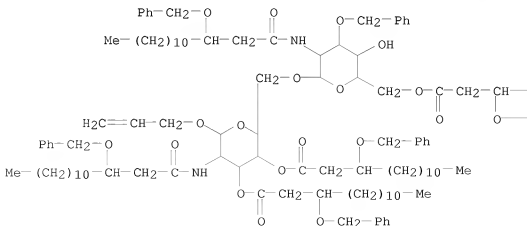
IT 87357-71-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(preparation and reaction of)

RN 87357-71-9 HCAPLUS

CN β -D-Glucopyranoside, 2-propenyl

2-deoxy-6-O-[2-deoxy-6-O-[1-oxo-3-(phenylmethoxy)tetradecyl]-2-[[1-oxo-3-(phenylmethoxy)tetradecyl]amino]-3-O-(phenylmethyl)-β-D-glucopyranosyl]-2-[[1-oxo-3-(phenylmethoxy)tetradecyl]amino]-, 3,4-bis[3-(phenylmethoxy)tetradecanoate], [2(R),3(R),4(R),6(2R),6(R)]-(9CI) (CA INDEX NAME)



$$\text{---}(\text{CH}_2)_{10}\text{---Me}$$
$$\text{---CH}_2\text{---Ph}$$

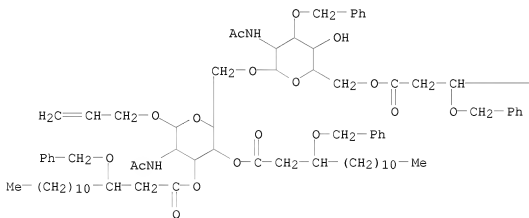
IT 88862-42-4P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and trichloroethoxycarbonylation of)

RN 88862-42-4 HCAPLUS

CN β -D-Glucopyranoside, 2-propenyl
2-(acetylamino)-6-O-[2-(acetylamino)-2-deoxy-6-O-[1-oxo-3-
(phenylmethoxy)tetradecyl]-3-O-(phenylmethyl)- β -D-glucopyranosyl]-2-
deoxy-, 3,4-bis[3-(phenylmethoxy)tetradecanoate], [3(R),4(R),6(R)]- (9CI)
(CA INDEX NAME)

PAGE 1-A

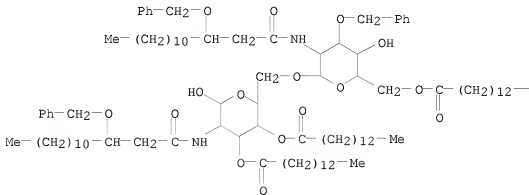


PAGE 1-B

$$-(\text{CH}_2)_{10}-\text{Me}$$

L33 ANSWER 37 OF 42 HCAPLUS COPYRIGHT 2008 ACS on STN
 TI Synthetic approach to lipid A: preparation of phosphorylated
 disaccharides containing (R)-3-hydroxyacyl and (R)-3-acyloxyacyl groups
 GI For diagram(s), see printed CA Issue.
 AB Seven lipid A analogs I [R1 = tetradecanoyl, (R)-3-hydroxytetradecanoyl;
 R2 = (R)-3-hydroxytetradecanoyl, (R)-3-tetradecanoyloxytetradecanoyl; R3
 and R4 = H, P(O)(OH)2] were prepared from disaccharide II in several steps.
 AN 1983:558753 HCAPLUS <<LOGINID::20081210>>
 DN 99:158753
 OREF 99:24353a,24356a
 TI Synthetic approach to lipid A: preparation of phosphorylated
 disaccharides containing (R)-3-hydroxyacyl and (R)-3-acyloxyacyl groups
 AU Inage, M.; Chaki, H.; Imoto, M.; Shimamoto, T.; Kusumoto, S.; Shiba, T.
 CS Fac. Sci., Osaka Univ., Osaka, 560, Japan
 SO Tetrahedron Letters (1983), 24(19), 2011-14
 CODEN: TELEAY; ISSN: 0040-4039
 DT Journal
 LA English
 IT 87374-34-3
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (phosphorylation of, with dibenzyl phosphorochloridate)
 RN 87374-34-3 HCAPLUS
 CN α -D-Glucopyranose, 2-deoxy-6-O-[2-deoxy-2-[[1-oxo-3-
 (phenylmethoxy)tetradecyl]amino]-6-O-(1-oxotetradecyl)-3-O-(phenylmethyl)-
 β -D-glucopyranosyl]-2-[[1-oxo-3-(phenylmethoxy)tetradecyl]amino]-,
 3,4-ditetradecanoate, [2(R),6[2(R)]]- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B

— Me

IT 87357-77-5P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)

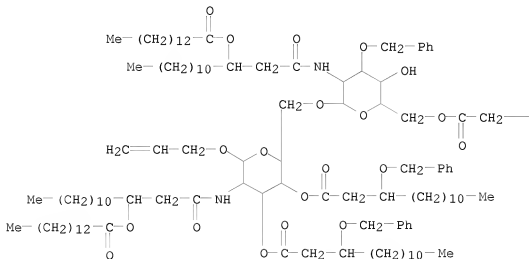
(preparation and deallylation of)

RN 87357-77-5 HCAPLUS

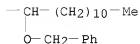
CN β -D-Glucopyranoside, 2-propenyl

2-deoxy-6-O-[2-deoxy-6-O-[1-oxo-3-(phenylmethoxy)tetradecyl]-2-[[1-oxo-3-[[1-oxotetradecyl]oxy]tetradecyl]amino]-3-O-(phenylmethyl)- β -D-glucopyranosyl]-2-[[1-oxo-3-[[1-oxotetradecyl]oxy]tetradecyl]amino]-, 3,4-bis[3-(phenylmethoxy)tetradecanoate], [2(R),3(R),4(R),6[2(R),6(R)]]-(9CI) (CA INDEX NAME)

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PAGE 1-B



IT 87357-71-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and deprotection of)

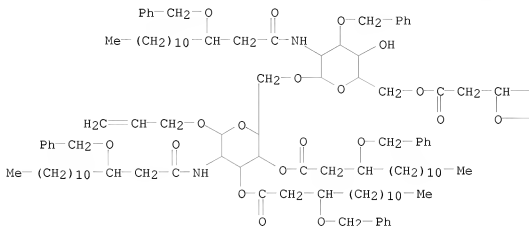
RN 87357-71-9 HCAPLUS

CN β -D-Glucopyranoside, 2-propenyl

2-deoxy-6-O-[2-deoxy-6-O-[1-oxo-3-(phenylmethoxy)tetradecyl]-2-[[1-oxo-3-(phenylmethoxy)tetradecyl]amino]-3-O-(phenylmethyl)- β -D-glucopyranosyl]-2-[[1-oxo-3-(phenylmethoxy)tetradecyl]amino]-,

3,4-bis[3-(phenylmethoxy)tetradecanoate], [2(R),3(R),4(R),6[2(R),6(R)]]-(9CI) (CA INDEX NAME)

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PAGE 1-B

— (CH₂)₁₀—Me

—CH₂—Ph

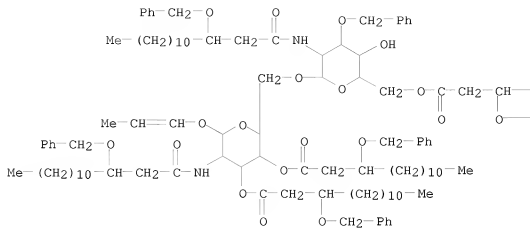
IT 87374-33-2P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and phosphorylation of, with Ph dihydrogen phosphate)

RN 87374-33-2 HCAPLUS

CN β-D-Glucopyranoside, 1-propenyl

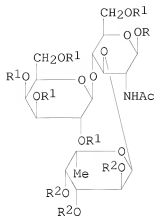
2-deoxy-6-O-[2-deoxy-6-O-[1-oxo-3-(phenylmethoxy)tetradecyl]-2-[[1-oxo-3-(phenylmethoxy)tetradecyl]amino]-3-O-(phenylmethyl)-β-D-glucopyranosyl]-2-[[1-oxo-3-(phenylmethoxy)tetradecyl]amino]-, 3,4-bis[3-(phenylmethoxy)tetradecanoate], [2(R),3(R),4(R),6[2(R),6(R)]]-(9CI) (CA INDEX NAME)



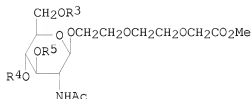
— (CH₂)₁₀—Me

—CH₂—Ph

L33 ANSWER 38 OF 42 HCAPLUS COPYRIGHT 2008 ACS on STN
 TI 3-Fucosyl-N-acetyllactosamine derivatives and their biological
 applications
 GI



I



II

AB The tile compds. I [R = (un)substituted alkyl, alkenyl; R1, R2 = H, protective group] were prepared for use as specific antigens and the manufacture of antibodies for the immunochem. detection of types of tumors. Thus HO(CH2CH2O)2H was O-benzoylated, treated with BrCH2CO2Et, and debenzylated to give HO(CH2CH2O)2CH2CO2Me which was treated with acetochloro-N-acetylglucosamine to give II (R3-R5 = Ac). Deprotection and reprotection of II (R3-R5 = Ac) gave II (R3 = Bz, R4 = H, R5 = CH2Ph) which was treated with 1-O-trichloroacetimidyl-2,3,4,6-tetra-O-acetyl- α -D-galactopyranoside and, after debenzylation, with 10-(N-methylacetimidyl)-2,3,4-tri-O-benzyl- β -L-fucopyranoside to give I [R = O(CH2CH2O)2CH2CO2Me, R1 = acyl, R2 = CH2Ph]. The latter compound was deblocked in 2 stages to give I [R = O(CH2CH2O)2CH2CO2Me, R1 = R2 = H].

AN 1983:471131 HCAPLUS <<LOGINID:20081210>>

DN 99:71131

OREF 99:11062h,11063a

TI 3-Fucosyl-N-acetylactosamine derivatives and their biological applications

IN Feizi, Ten; Gooi, Hock Chye; Sinay, Pierre

PA Choay S. A., Fr.

SO Eur. Pat. Appl., 47 pp.

CODEN: EPXXDW

DT Patent

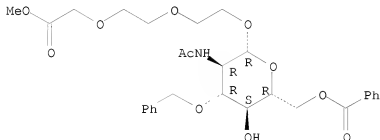
LA French

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 69678	A2	19830112	EP 1982-401292	19820708 <--
	EP 69678	A3	19830209		
	R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE				
	FR 2509313	A1	19830114	FR 1981-13447	19810708 <--
	JP 58015993	A	19830129	JP 1982-119136	19820708 <--
	US 4563445	A	19860107	US 1984-569487	19840109 <--
PRAI	FR 1981-13447	A	19810708	<--	

US 1982-396193 A1 19820708 <--
 OS MARPAT 99:71131
 IT 86520-62-9P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation and reaction of, with trichloroacetimidoyltetraacetyl-galactose)
 RN 86520-62-9 HCAPLUS
 CN Acetic acid, [2-[2-[[2-(acetyl-amino)-6-O-benzoyl-2-deoxy-3-O-
 (phenylmethyl)-β-D-glucopyranosyl]oxy]ethoxy]ethoxy]-, methyl ester
 (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L33 ANSWER 39 OF 42 HCAPLUS COPYRIGHT 2008 ACS on STN
 TI Glucosamine-peptide derivatives and their use
 GI For diagram(s), see printed CA Issue.
 AB Glucosamine peptides I [R = alkyl, hydroxyalkyl, aralkyl; R1 = H, acyl, cycloalkylacetyl; R2 = H, alkyl; m = 0, 1; n = 0-9; R3 = H, alkyl; R4, R5 = H, alkyl, hydroxyalkyl; R8, R9 = H, alkyl, aralkyl] were prepared and had immunostimulating, anti-infectious, and antitumor activity. Thus, acylating muramylvalylisoglutamate II with PhCH2O2C-Gly-OC6H4NO2-4 and then hydrogenolysis and acylating with nitrophenyl 10-(2,3-dimethoxy-5-methyl-1,4-benzoquinon-6-yl)decanoate gave muramyl peptide III. III at 100 μg inhibited growth of Meth-A tumor cells in mice 4 wk.

AN 1981:175559 HCAPLUS <<LOGINID:20081210>>
 DN 94:175559
 OREF 94:28711a
 TI Glucosamine-peptide derivatives and their use
 IN Yamamura, Yuichi; Azuma, Ichiro; Shigeru, Kobayashi
 PA Takeda Chemical Industries, Ltd., Japan
 SO Eur. Pat. Appl., 113 pp.
 CODEN: EPXXDW
 DT Patent
 LA English
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 14984	A1	19800903	EP 1980-100811	19800218 <--
	EP 14984	B1	19821201		
	R: AT, BE, CH, DE, FR, GB, IT, LU, NL, SE				
	JP 55111499	A	19800828	JP 1979-19929	19790221 <--
	JP 62044555	B	19870921		
	AT 1906	T	19821215	AT 1980-100811	19800218 <--
	US 4369178	A	19830118	US 1980-123401	19800221 <--
	CA 1239636	A1	19880726	CA 1980-346133	19800221 <--
PRAI	JP 1979-19929	A	19790221	<--	

EP 1980-100811 A 19800218 <--

OS MARPAT 94:175559

IT 77277-42-0P 77277-57-7P 77290-25-6P

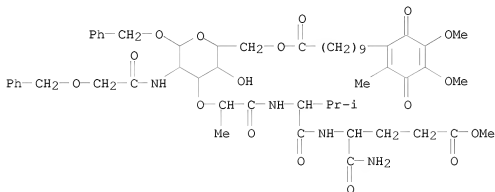
77290-27-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and hydrogenolysis of)

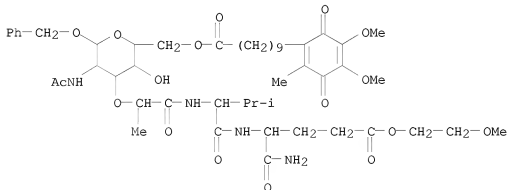
RN 77277-42-0 HCAPLUS

CN D- α -Glutamine, N2-[N-[6-O-[10-(4,5-dimethoxy-2-methyl-3,6-dioxo-1,4-cyclohexadien-1-yl)-1-oxodecyl]-N-[(phenylmethoxy)acetyl]-1-O-(phenylmethyl)- α -muramoyl]-L-valyl]-, methyl ester (9CI) (CA INDEX NAME)



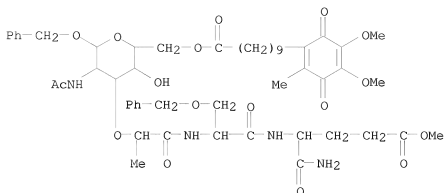
RN 77277-57-7 HCAPLUS

CN D- α -Glutamine, N2-[N-[N-acetyl-6-O-[10-(4,5-dimethoxy-2-methyl-3,6-dioxo-1,4-cyclohexadien-1-yl)-1-oxodecyl]-1-O-(phenylmethyl)- α -muramoyl]-L-valyl]-, 2-methoxyethyl ester (9CI) (CA INDEX NAME)



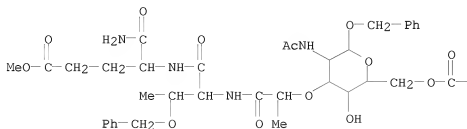
RN 77290-25-6 HCAPLUS

CN D- α -Glutamine, N2-[N-[N-acetyl-6-O-[10-(4,5-dimethoxy-2-methyl-3,6-dioxo-1,4-cyclohexadien-1-yl)-1-oxodecyl]-1-O-(phenylmethyl)- α -muramoyl]-O-(phenylmethyl)-L-seryl]-, methyl ester (9CI) (CA INDEX NAME)

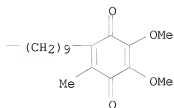


RN 77290-27-8 HCAPLUS
 CN D- α -Glutamine, N2-[N-[N-acetyl-6-O-[10-(4,5-dimethoxy-2-methyl-3,6-dioxo-1,4-cyclohexadien-1-yl)-1-oxodecyl]-1-O-(phenylmethyl)- α -muramoyl]-O-(phenylmethyl)-L-threonyl]-, methyl ester (9CI) (CA INDEX NAME)

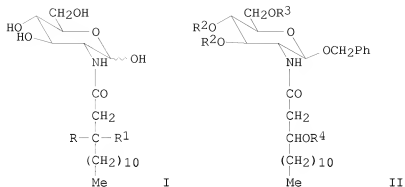
PAGE 1-A



PAGE 1-B



L33 ANSWER 40 OF 42 HCAPLUS COPYRIGHT 2008 ACS on STN
 TI A convenient synthesis of 2-deoxy-2-(D- and L-3-hydroxytetradecanoylamino)-D-glucose: diastereoisomers of the monomeric, lipid A component of the bacterial lipopolysaccharide
 GI



AB The title aminoglucosides (I; R = H, R1 = OH; R = OH, R1 = H) were prepared from diastereoisomeric glucopyranoside II (R2 = R3 = Ac, R4 = H) (III) in several steps. III was in sequence treated with MeO(CH2)2OCH2Cl, deacetylated, and tritylated at which stage the resultant isomers (ratio 1:1) D- and L-II [R2 = H, R3 = Ph3C, R4 = MeO(CH2)2OCH2] were separated by chromatog. on silica gel. The isomers were converted into the corresponding title compds. in 5 steps.

AN 1981:175404 HCAPLUS <<LOGINID::20081210>>

DN 94:175404

OREF 94:28679a, 28682a

TI A convenient synthesis of 2-deoxy-2-(D- and L-3-hydroxytetradecanoylamino)-D-glucose: diastereoisomers of the monomeric, lipid A component of the bacterial lipopolysaccharide

AU Kiso, Makoto; Nishiguchi, Hisao; Murase, Satoshi; Hasegawa, Akira

CS Dep. Agric. Chem., Gifu Univ., Kakamigahara, 504, Japan

SO Carbohydrate Research (1981), 88(1), C5-C9

CODEN: CRBRAT; ISSN: 0008-6215

DT Journal

LA English

IT 77364-30-8P 77364-31-9P

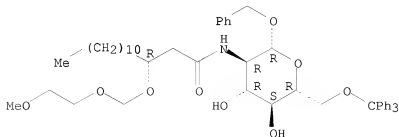
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and detritylation of)

RN 77364-30-8 HCAPLUS

CN β -D-Glucopyranoside, phenylmethyl

2-deoxy-2-[[3-[(2-methoxyethoxy)methoxy]-1-oxotetradecyl]amino]-6-O-(triphenylmethyl)-, (R)- (9CI) (CA INDEX NAME)

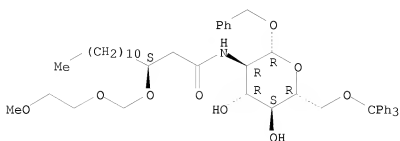
Absolute stereochemistry.



RN 77364-31-9 HCAPLUS

CN β -D-Glucopyranoside, phenylmethyl
2-deoxy-2-[[3-[(2-methoxyethoxy)methoxy]-1-oxotetradecyl]amino]-6-O-
(triphenylmethyl)-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L33 ANSWER 41 OF 42 HCAPLUS COPYRIGHT 2008 ACS on STN
TI Glucosamine peptide derivatives and their pharmaceutical compositions
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Acetylmuramyl dipeptide derivs. I [n = O, R = H, alkyl; n = 1-9, R = H, NH₂; R1 and R2 = alkyl; R3 and R4 = H, alkyl, CH₂OH; R5 and R6 = CO₂H, CONH₂; R7 = H, R8CO (R8 = acyclic hydrocarbon which can be ω -substituted by cycloalkyl), Q (l = 1-9; m = 0-9; t = 2-100; R8 and R9 = H, alkyl; R10 = alkyl, CO₂H which can be esterified, OH which can be etherified, pyrrolidino which can be substituted)] were prepared as immunostimulants. Thus, acetylmuramyl dipeptide II (R11 = H) was esterified with Z- β -Ala-OC₆H₄NO₂-p (Z = PhCH₂O₂C) to give II (R11 = Z- β -Ala), which was hydrogenated over Pd/C to give β -alanyl muramic acid derivative III (R12 = H) (IV). IV was N-acylated with CH₂:CMeCO₂Su (Su = succinimido) to give III (R12 = CH₂:CMeCO) (V), which was polymerized to give the homopolymer of V. V was copolymd. with N-vinyl-2-pyrrolidone, stearyl vinyl ether, and tridecyl methacrylate to give the resp. copolymers. The cell-mediated immunostimulatory activities of several I were tested.

AN 1980:198783 HCAPLUS <<LOGINID:20081210>>

DN 92:198783

OREF 92:32226h,32227a

TI Glucosamine peptide derivatives and their pharmaceutical compositions

IN Yuichi, Yamamura; Ichiro, Azuma; Shigeru, Kobayashi

PA Takeda Chemical Industries, Ltd., Japan

SO Eur. Pat. Appl., 80 pp.

CODEN: EPXXDW

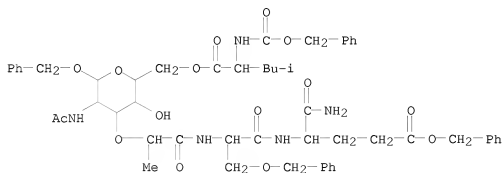
DT Patent

LA English

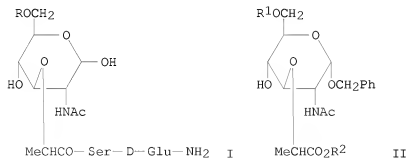
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 2677	A1	19790711	EP 1978-101524	19781202 <--
	EP 2677	B1	19821013		
	R: CH, DE, FR, GB, IT				
	JP 54079227	A	19790625	JP 1977-145415	19771202 <--

JP 54079228 A 19790625 JP 1977-145416 19771202 <--
 JP 02033719 B 19900730
 JP 54120696 A 19790919 JP 1978-28012 19780310 <--
 JP 63000446 B 19880107
 US 4430265 A 19840207 US 1982-393870 19820630 <--
 PRAI JP 1977-145415 19771202 <--
 JP 1977-145416 19771202 <--
 JP 1978-28012 19780310 <--
 US 1978-962033 A1 19781120 <--
 US 1981-249902 A1 19810401 <--
 OS MARPAT 92:198783
 IT 73341-32-9P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation and hydrogenolysis of)
 RN 73341-32-9 HCAPLUS
 CN D- α -Glutamine, N-[N-[N-acetyl-1-O-(phenylmethyl)- α -muramoyl]-O-
 (phenylmethyl)-L-seryl]-, phenylmethyl ester, 6'-ester with
 N-[(phenylmethoxy)carbonyl]-L-leucine (9CI) (CA INDEX NAME)



L33 ANSWER 42 OF 42 HCAPLUS COPYRIGHT 2008 ACS on STN
 TI Muramyl dipeptide derivatives
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AB Muramyl dipeptides I (R = mycoloyl, norcardomycoloyl) were prepared as antitumor agents. Thus, muramic acid II (R₁ = R₂ = H) was esterified with

AN 1979:611832 HCAPLUS <<LOGINID::20081210>>
DN 91:211832
OREF 91:34149a,34152a
TI Muramyl dipeptide derivatives
IN Yamamura, Yuichi; Shiba, Tetsuo; Azuma, Ichiro; Kusumoto, Shoichi;
Hirayama, Tadachika; Hiba, Tsuneo
PA Daiichi Seiyaku Co., Ltd., Japan
SO Jpn. Kokai Tokkyo Koho, 8 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT.1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 54073729	A	19790613	JP 1977-137088	19771115 <--
	JP 60033120	B	19850801		
PRAI	JP 1977-137088	A	19771115	<--	
IT	71921-85-2DP, 6-O-mycoloyl derivative				
	RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)				
	(preparation and hydrogenation of)				
RN	71921-85-2 HCAPLUS				
CN	D-α-Glutamine, N2-[N-[N-acetyl-1,6-bis-O-(phenylmethyl)-α-muramoyl]-O-(phenylmethyl)-L-seryl]-, phenylmethyl ester (9CI) (CA INDEX NAME)				

